

Germanium and GeSn based Quantum Well Lasers and Nanoscale Multi-gate FETs

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ABSTRACT (Academic)

The incredible technological advancements over the last century have been possible due to *tiny trinkets* designed using semiconducting crystalline materials, especially Silicon and III-V compounds. Silicon, a group IV element has become the first choice in developing microchips serving an ever-growing set of applications including, computation, RF communications, solar cells, power electronics, quantum computing and its periphery, optoelectronics, IOT sensors, and lately artificial intelligence. Billions of Si-based complementary transistors (CMOS) are present at the center of most computing devices used today such as HPC servers, compute farms, laptops, and smartphones. The astonishing rise in transistor count, performance, and functionality as well as the exponential reduction in cost has been possible over the past decades due to a singular idea: shrinking the device. However, this rule, also called *Moore's Law* has been slowing over the past two decades and has eventually come to a standstill in its traditional definition. Moore's law has since been sustained by ingenious innovations such as high-k gate dielectrics, vertical scaling, lattice strain engineering, novel material developments and, lately chiplets as well as multi-die vertical packaging. As conventional Si CMOS approaches a roadblock, this work presents research on Germanium-based multi-gate devices providing promise for faster and low-power operation. This work discusses how Ge grown on a GaAs substrate can be tuned and utilized to form a virtually defect-free channel for ultra-scaled multi-gate transistors. Calibrated solvers informed using in-house materials and devices as well as literature are used to predict device performance for advanced structures. Further, a hybrid CMOS system with the high hole mobility p-channel device formed using tensile strained Ge, and the high electron mobility n-channel device formed using the underlying InGaAs layer is proposed and simulated. As scaling approaches Gate-all-around Nanosheet FETs in 2024 and complementary-FETs (CFETs) around 2034, Ge-on-AlAs based transistors can offer unique process simplifications, defect reduction, yield improvement, and high-performance advantages showing promise for future IRDS nodes. The process design,

material stack, device, and circuit performance for this novel Ge-based NSFET is presented in this work. The lack of large strain or strain relaxation in the NS multilayer starting stack is seen to be a great process advantage for the Ge-AlAs NSFET system.

To a certain extent, Si seems omnipotent for all things electronics. However, one exception is on-chip light generation. A coherent electrically controllable on-chip light source is a central component critical for optoelectronics, quantum technologies, fiber communications, and sensing. Due to the indirect bandgap, Si cannot produce light hence direct bandgap materials such as GaAs and GaN have been the primary choice for off-chip light sources integrable on the platform. Interestingly, Ge has a pseudo-direct bandgap, i.e., unlike Silicon, it can be manipulated to produce light using heavy doping, tensile strain, and Sn alloying. Similar to conventional III-V light sources, reduction in the dimensionality of the gain medium, i.e., Ge can enable a drastic reduction in the current required to produce light, among other performance considerations. This reduced dimensionality can be achieved by forming quantum wells and quantum dots. In this work, two new types of Ge-based quantum well lasers are introduced and analyzed along with qualitative and quantitative benchmarking. The first QW laser uses a small epitaxial biaxial tensile strain to improve the *direct-ness* of the Ge gain medium. The internal quantum efficiency, net gain, and threshold current can be improved drastically by choosing the right tensile strain while staying within a certain critical thickness value. For the first time, the impact of biaxial tensile strain on the optical properties of Ge is analyzed and reported through a systematic study of the dielectric spectra and optical constant using VASE. The changes in the band structure due to tensile strain are correlated with the critical points to uncover various optical transitions. An even better QW laser architecture is possible by utilizing a GeSn QW. This QW laser uses Sn-alloying to form a GeSn active region which is further lattice matched to the waveguide (InGaAs) and the optical confinement layers (InAlAs) around it. This completely lattice-matched laser structure can offer unique advantages such as virtually defect-free active region, tunability as well as improved efficiency and threshold current density. The absence of strain and consequently strain relaxation in the laser stack enables one to steer away from the critical thickness limitation while opening doors to designing multiple quantum well lasers among other complex architectures. The impact of Sn alloying on the atomic structure, lattice coherence, and relaxation is analyzed through XRD reciprocal space maps and rocking curves as a function of Sn concentration. Further, this lattice-matched system, GeSn-

InGaAs-InAlAs has the potential to mirror the benefits of the mature GaAs-AlGaAs system which led to many great technological innovations over the past decades such as lasers and LEDs.

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ABSTRACT (General Audience)

The incredible technological advancements over the last century have been possible due to *tiny trinkets* designed using semiconducting crystalline materials, especially Silicon and Group III-V alloys. These semiconductor devices have been used to make scalable computers, sensors, memory storage systems and many more revolutionary technologies. These devices can be broadly classified as light-based devices such as lasers/LEDs (usually dominated by group III-V materials) and current-based devices such as transistors (largely dominated by Si). This thesis introduces two transistor technologies to extend the scaling beyond conventional Si devices into the next decade. Through calibrated numerical solvers, a high mobility Ge and InGaAs cointegrated CMOS system for 0.5 V is introduced, analyzed and benchmarked with literature. A lattice matched Ge-on-AlAs multilayer stack is shown to have great potential to form a novel CMOS system which uses Ge Nanosheets, providing process advantage and superior performance. The next part of the thesis, dealing with the light-based devices, introduces two types of Ge based quantum well lasers, one based on tensile strained Ge and the other based on lattice matched GeSn. Both show large performance improvements over previous attempts in literature. Lasing from an indirect bandgap material such as Ge, the associated challenges and performance metrics are discussed. Lastly, the optical, dielectrics and critical point properties of tensile strained Ge are presented for the first time uncovering interesting physical trends. Ge samples with increasing tensile strain are grown using MBE and measured using ellipsometry to elucidate the physical phenomenon.

Acknowledgments

As I complete an important milestone, I would like to look back and thank all the people in my life who have been instrumental to my journey.

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Most importantly, I would like to thank my parents, who have supported me in all the major decisions in my life, from Pune to Delhi to Bangalore and Blacksburg. Through all the good times and the bad, they have kept me grounded and locked in on my path. My mother through her calm energy, scientific research mindset, and patience, and my father through his humor, greater vision, and confidence. I would like to thank my family and friends, for believing in my abilities and supporting me. I would like to thank my wife, Shimoli, for being there by my side through the last few years as we navigated interesting and challenging circumstances.

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Contributions through this work

This work provides solutions to two questions enabling advancement of semiconductor devices such as transistors and quantum well lasers. Can Germanium become a Beyond Moore solution for extending the transistor roadmap beyond traditional Si devices? Can Ge and GeSn form quantum wells for efficient laser operation in the MIR spectral range enabling classical and quantum on-chip applications? The solutions to these questions are presented methodically to the scientific community through journal publications and international conferences ensuring readability, understandability, reproducibility, and simplicity. As a part of this dissertation and the research carried out over the past few years, I have made the following contributions to the subject of semiconductor transistor devices and semiconductor quantum well lasers:

1. Alternate channel CMOS material-to-device-to-circuit co-optimization for a ***tensile Ge on InGaAs-based FinFET system***. This monolithic system operated at 0.5 V supply while providing a high electron mobility InGaAs n-channel as well as a high hole mobility Ge p-channel. An interesting discussion of material and quantum properties on the CMOS circuit level performance is presented. The extensive tunability and design considerations of this system by varying the tensile strain through the Indium composition are presented for the first time. Thus, introducing a completely new type of hybrid dual material high-performance low-power CMOS, for beyond Silicon explorations.
2. Germanium grown lattice-matched on AlAs can form multi-layer structures suitable for advanced ***Angstrom era high mobility Ge Nanosheet-FETs***. This work introduces a novel CMOS system for beyond-Moore electronics leveraging Ge grown on a lattice matched sacrificial AlAs. The AlAs can act as a sacrificial layer during the process, resulting in superior etch selectivity compared to existing processes while acting like a conduction barrier. The process variation immunity is seen to be a huge advantage for yield and reliability. The LM Ge layers can be defect-free resulting in reliable operation and high yield. Potentially, this system can provide a process/manufacturability advantage over its Si counterparts, something that never existed before. The material-

to-device-to-circuit co-optimization for this monolithic LM system is discussed while evaluating the performance at advanced nodes. This Ge NSFET system can prove to be a suitable candidate for advanced Angstrom-era nodes, ensuring device and performance scaling beyond 2034.

3. Light emission is possible only from direct bandgap materials like GaAs, not from indirect bandgap materials like Si and Ge. This work dives deep into the fundamentals of semiconductor lasers to introduce a new type of laser that enables lasing from Ge, an indirect bandgap material. A ***Ge based Quantum well laser*** is introduced, through novel theory and experiments, that utilizes the underlying InGaAs layer as a strain template and QW barrier as well as the waveguide. The performance of such a monolithic laser is seen to be orders of magnitude better in terms of threshold current density, IQE, and net gain, compared to previous Ge laser reports. Through experiments, the band alignment and minority carrier lifetime is determined for multiple samples and fed to the numerical solvers. A detailed theoretical framework specific to tunable tensile Ge lasers and waveguides is built and metrics are evaluated. Such a laser, made using a Ge quantum well can have a wide range of applications suitable for classical and quantum technologies, sensing, and communication.
4. Biaxial epitaxial tensile strain can have interesting implications for Ge-based devices such as lasers. The impact of ***biaxial epitaxial tensile strain on the optical and dielectric constants of Ge*** have been measured for the first time through this work. The optical constants n (refractive index), k (extinction coefficient), and absorption coefficient as well as the dielectric constants such as ϵ_1 and ϵ_2 are evaluated for multiple tensile strained Ge samples grown on a composition-controlled InGaAs LGB and InGaAs strain template. The samples are grown using MBE and analyzed using VASE. Interesting physical phenomena associated with the movement of the band energies, spin-orbit coupling, and band structure due to the tensile strain are uncovered through critical point analysis in this work. This is the first report of the impact of tensile strain

on dielectric and optical constants as well as CPs of epitaxial thin film Ge, this can enable better design and analysis of optoelectronic devices based on Ge.

5. A new ***lattice matched GeSn-InGaAs quantum well laser*** system is explored through this work. This monolithic system where the entire separate-confinement-heterostructure for the quantum well laser structure utilizes three semiconductors (GeSn, InGaAs, InAlAs), all of which can be designed to be atomically “cooperative” *i.e.*, lattice matched. The methodology to do so is introduced in this work, along with the design considerations and performance qualifications. Further, alloying Ge with small percentages of Sn can enable better optical emission from GeSn. This LM system can have benefits previously seen for the GaAs-AlGaAs laser system, which led to great technological innovations owing to the special material properties such as LM and band offsets. The proposed GeSn laser stack provides these advantages, LM and band offsets, along with a few others. This laser can achieve ultra-low threshold current density at $\sim 14\%$ Sn composition as well as a good operating range between 8 - 18% Sn. The wide tunability for classical and quantum applications, as well as the excellent performance and manufacturability, make this laser an enticing avenue for future exploration.

List of Publications

- [1] **R. Joshi**, S. Karthikeyan, and M. K. Hudait, "Monolithically Cointegrated Tensile Strained Germanium and In_xGa_{1-x}As FinFETs for Tunable CMOS Logic," *IEEE Trans. on Electron Dev.*, vol. 69, no. 8, pp. 4175-4182, Aug. 2022, doi: 10.1109/TED.2022.3181112.
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- [3] **R. Joshi**, S. Karthikeyan and M. K. Hudait, "Germanium Nanosheet-FETs Scaled to Subnanometer Node Utilizing Monolithically Integrated Lattice Matched Ge/AlAs and Strained Ge/InGaAs," *IEEE Trans. on Electron Dev.*, vol. 70, no. 3, pp. 899-907, March 2023, doi: 10.1109/TED.2023.3238376.
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- [10] Rebecca Rainhart, Purv Bavishi, Ben Westcott, Zibing He, **Rutwik Joshi**, and M. K. Hudait, "*Adaptive Design of Tensile Strained Ge-on-InGaAs QW Laser for MIR Applications*", 8th IEEE Electron Devices Technology and Manufacturing (EDTM) Conference 2024, March 3-6 (2024). 2024 IEEE EDTM, Bangalore, India, March 3-6 (2024)
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Chapter 1 – Introduction, History and Overview

1.1 Evolution of the transistor and the digital technology roadmap

Since the development of the first transistor and the first integrated circuits in the late 20th century, the structure and operation of the *unit cell of digital computation*, *i.e.*, the Metal-Oxide-Semiconductor Field Effect Transistor (MOSFET) has been nearly fixed. A voltage is applied at the gate to control the conductivity of the channel between an ON-state and an OFF-state, which represent the two states of this switch. An ideal switch would allow no current to pass in the OFF-state and provide no resistance to current in the ON-state. But, in reality, a MOSFET offers a finite resistance in both the states and the design challenge is to ensure that the ratio of ON-current and OFF-current is large enough. This motivates the need to define certain metrics and specifications for the operation of a real MOSFET. As a device designer and semiconductor physicist, the objective is then to engineer a device such that, (i) consumes little power, (ii) meets area, current, and voltage performance specifications, (iii) the process is scalable to billions, (iv) materials are affordable, (v) manufacturing is easy and reliable, and (vi) devices operate tolerably for years. With the exponentially growing need for compute, data, and memory every year, the MOSFET needs to get smaller, faster, and more power efficient every year. In retrospect, since the first integrated MOSFET circuits, (i) the number of transistors on a chip has grown from roughly 10 to 10 billion, (ii) the individual transistor feature size has reduced roughly by 25000x moving from the sub-mm regime to the deep sub-micron technologies today, (iii) memory bit storage and usage has grown from a few bits to terabits today, (iv) the size of a typical computing unit or a CPU has shrunk from an entire room to the palm of your hand, and (v) power efficiency has improved by orders of magnitude. Integrated circuits have come a long way, but the need for better power efficiency, speed, and compactness is ever-growing and exponential.

To meet this ever-growing need for compute, memory, and storage the MOSFET performance metrics need to be evaluated and optimized. Critical device level metrics are, (i) ON-current I_{ON} which is also an indicator of the resistance offered by the device in the ON-state, (ii) OFF-current I_{OFF} which is the ability of the device to block current in the OFF-state to avoid

leakage, (iii) ratio of I_{ON} and I_{OFF} , (iv) subthreshold swing (SS) an indicator of the smallest gate voltage required to increase the drain current by 1 order of magnitude, (v) drain induced barrier lowering (DIBL) an indicator of the unwanted influence of the drain voltage on the gate, (vi) source and drain resistance, (vi) threshold voltage for the switching, (vii) gate oxide quantum tunneling leakage, and (viii) area consumed. These device-level metrics in turn determine the circuit and system-level performance specifications. At the circuit and system level, one important metric is the total power consumed,

$$P = n(CV_{DD}^2 f + I_{OFF}V_{DD}) \quad (1.1)$$

where the first term indicates the dynamic power consumption, and the second term is associated with the static leakage. A clear dependence on the supply voltage is seen indicating that reducing the power supply voltage can have a significant impact on reducing the total chip power consumption. The frequency of switching denoted by f also has a linear dependence indicating that faster computation speed and faster switching will increase the dynamic power dissipation. With the growing need for computations and speed, decreasing the switching frequency is not a viable solution. Most applications today demand an ever-increasing clock frequency approaching a few GHz. Furthermore, the number of transistors n in the module or the chip also scales the power consumed in a linear fashion. Again, due to the exponentially rising functional units on a module, reducing the number of transistors is not a viable option. A popular solution employed in most modern ICs today is power management units, which help reduce the number of active functional units by utilizing a sleep feature, thus reducing the effective value of n . The output load capacitance C which the module drives has two components: the internal parasitic capacitance of the MOSFET terminals and the fan-out number i.e., the gates and loads to be driven by the gate. Reducing device geometries (area) associated with the active regions can help reduce the parasitic internal capacitance of all gates enabling faster and lower power operation. But this comes at the cost of drive strength and parasitic resistance. Lastly, transistors and gates that are not operational or switching are expected to consume no power, but due to the leakage (I_{OFF}) devices dissipate power even in the off state. Additionally, there are other circuit performance metrics besides P , C , f , and n such as, (i) symmetric response, (ii) rise and fall time, (iii) delay, (iv) noise margin, and (v) area/layout.

1.2 Germanium: A high mobility channel for advanced multi-gate transistors

The search for novel materials and device architectures to improve upon existing Si-based transistors requires a consideration of the trade-off between the device/circuit performance and manufacture feasibility. The scaling of conventional Si complementary metal-oxide-semiconductor (CMOS) device feature size faces several technical challenges, including minimization of off-state leakage current (I_{OFF}); maintaining high drive current (I_{ON}) for circuit fan-out and high-speed operation; and supply voltage (V_{DD}) scaling to reduce total power dissipation and increase performance per watt while maintaining good noise margins. *In this work*, an approach to optimize and improve the device metrics beyond Si devices at the end of the roadmap [1] is developed, while using the circuit-level evaluations as boundary conditions for co-optimization. Investigations include gate architectures such as gate-all-around, nanotubes and nanowires [2,3] as well as channel architectures such as tunnel field effect transistors (TFETs), based on band-to-band tunneling and impact ionization MOS (IMOS) transistor, based on the avalanche breakdown providing extremely low subthreshold-swing (SS) at the cost of I_{ON} and reliability, respectively [3, 4]. However, the continued Si CMOS scaling has been possible with fully-depleted, raised-channel 3D fin transistor architectures that improve gated channel control and allow for sub-10 nm lateral down-scaling (fin width) through corresponding vertical up-scaling (fin height), while utilizing high- κ dielectric as the gate oxide [5]. Beyond this, researchers are investigating ultra-low power logic using high mobility materials (InGaAs and Ge) along with ultra-low equivalent oxide thickness (EOT). Over the years, several combinations of these architectures were investigated [6-16].

Germanium (Ge) is an attractive candidate for future nanoscale transistors due to its low bandgap of 0.67 eV and higher electron ($2\times$) and hole ($4\times$) mobilities compared to Si. Indeed, high-performance CMOS circuits leveraging Ge p- and Si n-FinFET have been demonstrated, where the Ge layer was transferred to a 300 mm Si wafer [6] since the direct epitaxy of Ge on Si suffers from a large lattice mismatch ($\sim 4.2\%$) induced defects and dislocations as well as low band offsets [7]. To circumvent the lattice mismatch-induced defects, wafer bonding, and Smart Cut™ techniques have been reported for the integration of alternate channel (Ge and III-V) CMOS circuits [8, 9]. However, layer transfer and wafer bonding are expensive and thus, the large-scale integration of logic devices proves to be challenging in terms of voids, wafer alignment, cost, and

density [10]. On the other hand, InGaAs on oxide-on-insulator (OI), InAs-OI, Ge-OI, and SiGe-OI based transistors have been studied through simulations [11,12] and experiments [8], [13]. The growth of such semiconductor layers on -OI wafers enables access to high electron mobility materials but poses an issue of thermal conductivity mismatch that can result in defects, cracks, and unintentional strain on the active layers. Thus, successful integration of Ge p-FET and high electron mobility $\text{In}_x\text{Ga}_{1-x}\text{As}$ n-FET would be a more viable option for monolithically co-integrated alternate channel CMOS logic [13].

Chapter 3 discusses the device and circuit simulations of monolithically co-integrated alternate channel CMOS device architecture consisting of tensile strained germanium ($\epsilon\text{-Ge}$) for the p-channel FinFET and variable indium (In) compositional $\text{In}_x\text{Ga}_{1-x}\text{As}$ ($0.10 \leq x \leq 0.53$) for the n-channel FinFET. We study this $\epsilon\text{-Ge}/\text{InGaAs}$ co-integrated system in a FinFET gate architecture that provides significant electrostatic control over the channel in comparison to conventional MOSFET while being a reliable architecture that has been in industrial production for almost a decade (22 nm node – 5 nm node). The device simulation models were calibrated with the experimental Ge p-FinFET and InGaAs n-FinFET, and subsequently transferred to the co-integrated $\epsilon\text{-Ge}/\text{In}_x\text{Ga}_{1-x}\text{As}$ layer structure. The device parameters V_T , I_{ON} , I_{OFF} , and SS were evaluated for identical fin dimensions for n- and p-channel FinFETs as a function of In composition that alters the tensile strain in Ge. The threshold voltage (V_T) can be adjusted by varying the In composition in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer since the bandgap is different for each In composition and also in the upper $\epsilon\text{-Ge}$ layer. The V_T of $\text{In}_x\text{Ga}_{1-x}\text{As}$ n-FinFET and Ge p-FinFET can be tuned by the In composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$ during heteroepitaxial growth of the proposed $\epsilon\text{-Ge}/\text{In}_x\text{Ga}_{1-x}\text{As}$ structure, whereas in conventional Si CMOS process, the doping adjustment to tune V_T is performed via ion implantation requiring additional process consideration [14]. This enables the use of a fixed photolithography process to generate tunable CMOS performance by varying In composition. In addition, the co-integrated CMOS inverter and ring oscillator performance for a supply voltage of 0.5 V are evaluated, and we show that the performance is noise-immune, symmetric, power-efficient as well as tunable for a wide range of In compositions.

Moving to lower dimensions closer to the N5 node is possible for this Ge p-FinFET and InGaAs n-FinFET cointegrated monolithic CMOS system, with distinct performance benefits and design considerations. Consequently at these scaled dimensions, a rigorous study of device metrics such as V_{TH} , I_{ON} , I_{OFF} , SS, and DIBL and their dependence on material parameters (*i.e.*, indium

composition, tensile strain, doping) and geometrical parameters (*i.e.*, channel length L , fin width W , and fin aspect ratio AR) using self-consistent analytical solvers, which capture realistic physics of nanoscale devices, is presented to characterize architectures scaled down to the N5 node [1]. Furthermore, in nanoscale multi-gate devices, the quantum confinement (QC) of inversion charge results in an additional capacitance in series with the oxide capacitance due to the charge centroid. This effect manifests in FETs as an increase in V_{TH} creating a challenge for device operability and scaling. The increase in V_{TH} results in a drop in I_{OFF} and a corresponding increase in I_{ON}/I_{OFF} ratio, while reducing SS and DIBL due to improved electrostatic control owing to QC. This performance consideration is valid only down to a specific width, beyond which the device transitions back to charge-dominated regime. An analysis to quantify this transition width (W_T) in the context of CMOS operability to be < 6 nm for $In_xGa_{1-x}As$ n-FinFET and ~ 20 nm for ϵ -Ge p-FinFET and illustrate the corresponding transition in design considerations for ultra-scaled CMOS devices.

Chapter 4 discusses how this Ge epitaxial system can fit well even beyond the N5 node in the IRDS roadmap as the transistor architecture moves from tri-gate FinFET devices to quad-gate gate-all-around Nanosheet-FET (NSFETs). Beyond the 3 nm FinFET node, further reduction in device footprint as well as improvement in device performance is possible by transitioning from FinFET to a gate-all-around (GAA) architecture [1]. In addition to the improved electrostatics provided by the GAA architecture, a vertical 3D stacking of devices is required to improve the chip integration density as well as individual device performance. As the industry unveils one of the first Si GAA-based designs [15]-[17], one must look for alternative design and process solutions to ensure sustained scaling of this technology to future high-performance and low-power computing. Approaching atomic dimensions aggravates pre-existing issues such as quantum confinement-induced changes in the bandgap, effective mass, and mobility as well as short channel effects (SCE): drain-induced barrier lowering (DIBL) and subthreshold swing (SS). The GAA nanosheet FET (NSFET) can be fabricated using the existing process and design infrastructure of the FinFET while providing a performance boost with a higher effective width [15]-[17]. In addition, the variability of the NS thickness is minimal as it is determined during epitaxy, whereas the fin height is determined by etching, thus making the NSFET performance more reliable and immune to random variations [15].

There are at least five ways to improve the drive capabilities of NSFET-based CMOS devices: alternate/modified channel material, parallel connection of multiple devices, wider

device, thicker sheet, and higher number of vertically stacked NS (N). Each of these, except the last, are design constraints shared with the FinFET and all of them have distinct effects on the performance of scaled NSFETs in terms of parasitics, threshold voltage (V_{TH}), SS, DIBL, I_{ON} , and I_{ON}/I_{OFF} ratio, while posing unique process and design challenges. One of the reasons for the success of Si-based p-FinFET over the years has been the high hole mobility for the (110) orientated crystallographic plane, resulting in improved performance of taller fins [18]. As we approach shorter and wider channel devices, like the Si NSFET or nanowire-FET (NWFET), this advantage will be lost due to the lower surface area of (110) plane, this warrants the use of higher hole mobility channel material. Germanium offers $4\times$ higher hole mobility than Si and exploration of Ge-based NSFET with higher hole mobility [5,19, 20] will provide superior device performance. Furthermore, the fabrication of Si NSFETs relies on a Si/SiGe multilayer epitaxial growth following a SiGe graded buffer, which results in a tensile strain ($\sim 1 - 1.5\%$) in the stack due to significant lattice mismatch between Si and the $Si_{0.7}Ge_{0.3}$ layer [21]. Although this strain may benefit device performance, it introduces a crucial constraint on the height of the device as well as the number of vertically stacked layers. Beyond a specific height, called the critical layer thickness, the pseudomorphic stack starts to relax the strain, resulting in an exponential rise in defects and dislocations [21]. In addition, the sacrificial layer, *here* $Si_{0.7}Ge_{0.3}$, should provide a high etch selectivity with respect to the active Si channel to ensure minimal loss of Si during fabrication [16]. Thus, along with a Ge channel for higher hole mobility, a Ge p-NSFET process that provides lattice-matched epitaxial growth as well as superior etch selectivity between active Ge layers and the sacrificial layers is required. Recently, Ge/SiGe epitaxial growth-based investigations for Ge p-GAA FETs have been reported through simulations as well as by experiment [16], [22-25].

This work explores a system that provides lattice-matched Ge/AlAs NS multilayer epitaxial growth, which can allow performance improvement through all the pathways discussed above as well as performance improvement over existing FinFETs. In addition, we show that vertical stacking of Ge NS is the most area and delay efficient pathway for improving CMOS circuit performance at advanced nodes such as the N0.7 node. Further, the wet-etch (vapor etch) of the AlAs using HF/BOE can provide a much superior etch selectivity than existing Si/SiGe systems, which rely on a directional dry-etch process with limited chemical selectivity.

The search for novel materials and device architectures to improve upon existing Si-based transistors requires consideration of the trade-off between the device/circuit performance and

manufacture feasibility. Further, a circuit-device-material co-optimization methodology is required to build the best possible *CMOS units* for the specific applications. Thus, a discussion about a new CMOS technology needs to proceed through rigorous analysis on 5 fronts:

1. **Material development and characterization:** Crystal growth, defect analysis, optical analysis (VASE, XRD, TEM), design of grading buffers, etc.
2. **Device design and simulation:** Extensive numerical simulations using calibrated solvers, quantification of device metrics and trends, the inclusion of non-ideal effects, heating, contacts, dopant diffusion, tunneling, leakage, *etc.*
3. **Device level process design:** A manufacturable, feasible, and cost-effective CMOS fabrication process needs to be visualized, simulated, and tested. Analysis related to process considerations such as chemical selectivity, deposition rates, surface orientations, thermal budget, etch rate, etc need to be evaluated to ascertain CMOS compatibility.
4. **Standard cell level circuit simulation:** Numerical characterization of circuit metrics, transients, parasitic effects, leakages, and loading. Co-optimization with device metrics to improve performance. Quantification of true standard cell level advantage for the proposed technology.
5. **Prototype device fabrication:** Utilizing the designed process to fabricate prototype devices followed by device probe testing, yield analysis, temperature-dependent IV-CV, and SEM/TEM imaging.

Analysis, quantitative and qualitative results as well as discussion on all 5 fronts will be provided in each of the following chapters in the context of novel semiconductor device development.

1.3 Technological revolution of the on-chip light sources

From the discovery and demonstration of the first p-n junction diodes, the path for a wide range of applications spanning sensing, electronics, computation, optical communication, *etc* has been laid. Since then Silicon has dominated most of the semiconductor electronics space, but it lacks a critical attribute that is indispensable for fiber communication, optoelectronics, and sensing. This critical attribute is the ability to generate light. Here, III-V compound semiconductors and their ability to generate light proved to be a game changer, resulting in the development of efficient lasers, LEDs, and detectors. The principles and fundamental conditions for the generation of light from a semiconductor material were initially presented by Bernard and Duraffourg in 1961 [26]. The first semiconductor lasers were reported within a span of 30 days by 4 groups parallelly in 1962. Important reports and developments followed, including emission studies from a GaAs junction in 1963 [27], analysis of stimulated emission and visible light generation from GaAs [28, 29], development of the heterostructure for confinement by Kroemer with the GaAs-AlAs system [30], the stripe structure using an oxide to form a laser ridge [31], quantum confinement in the well and threshold characteristics of a quantum well laser [32,33]. Extensive research on developing AlGaAs-InGaAs-InP based separate confinement heterostructure based lasers, material growth, theoretical framework, gain/threshold calculation, and design optimizations were reported over the years by the Yariv (CalTech) Group [34-36]. These works along with theoretical, experimental, and mathematical frameworks developed for laser waveguide design, strain engineering, band engineering, cavity design, optical mode solutions, quantum effects, defect engineering, recombination physics, carrier transport, as well as device engineering [37-39] has propelled lasers and LEDs into a mainstream commercially viable and accessible product today. Laser and LEDs made using these guidelines have emerged as indispensable components of lighting, optical research, quantum engineering, fiber communication, sensing, visible/IR imaging, and medical advancements.

1.4 Ge and GeSn based monolithic lasers: Challenges and Opportunities

After a brief review of the development of lasers over the years as well as the importance of these on-chip light sources, this section explores the possibility of using Ge as a light source. Beyond the age of electronic transistor technology, the future of computing and communication is possible through quantum technologies and photonics. These technologies are presently faced with some key challenges two of which are related to electronic-photonic monolithic integration and interfacing, and silicon (Si) compatibility of multi-material technologies for scaled production. At the center of quantum computation, sensing, and photonics lies an electrically powered coherent light source, and the ability to integrate such a light source with Si-compatible technologies on a chip has long been sought. In recent years, Ge is gaining popularity in photonic and optoelectronic devices [40], whereas $\text{In}_x\text{Ga}_{1-x}\text{As}$ has already gained popularity in optoelectronic applications [41,42]. Thus, integrating Ge and InGaAs-based logic devices in conjunction with optical devices (lasers, photodetectors, and interconnects) would be a step closer to the long-standing dream of an integrated optoelectronic chip [43-45].

Tensile strained germanium ($\epsilon\text{-Ge}$) is a potential candidate for such a coherent light source for several reasons: (i) the direct bandgap of Ge could provide ~ 1550 nm wavelength resulting in better compatibility with existing Si photonics and optical communication platforms [43, 44], (ii) strain induced tunable bandgap Ge [40, 46], (iii) compatibility with modern Si-based electronics fabrication infrastructure, and (iv) ability to form high-performance electronics [46] to drive the light source and interface with external circuitry. The benefits of the rapidly growing quantum technologies can be leveraged, provided a wide range of quantum elements made from different materials and systems can be co-integrated to form a heterogeneous chiplet-based system for achieving quantum supremacy [47]. Such a heterogeneous integration is a major challenge, and the complexity and cost of the process and system can be reduced significantly if the individual elements are compatible with existing Si infrastructure. This monolithically integrated Ge-based laser tunable in the $1.55\text{-}4\mu\text{m}$ range can find a wide set of applications such as day-time quantum key distribution [48, 49], resolving capacity crunch moving to $2\text{-}4\mu\text{m}$ for fiber communication spectrum [50], reduced linear and nonlinear losses [51] for integrated Si optics, quantum metrology, and sensing [52, 53], direct probing of the fundamental absorption bands of nearly all gas molecules [54]. The details of the experimental and theoretical investigation of the tensile

strained Ge SCH QW laser are discussed in **Chapter 5**. Before delving into the specific theory and details of the Ge laser technology, **Chapter 5** first explains in detail the framework for light generation, band structure, lasing, quantum wells, gain, threshold, waveguide design, and SCH to equip the reader with the fundamentals needed to understand the Ge laser discussion.

Following a detailed discussion of the application of tensile Ge epi-layers in quantum well lasers, it is crucial to measure and understand the optical and dielectric constants of Ge as the biaxial tensile strain gradually increases. **Chapter 6** discusses VASE measurements, absorption coefficients, critical point analysis, and optical constants of tensile Ge and the impact on the band structure. Among many interesting revelations about the optical spectra of tensile Ge, the apparent value of the E_0 spin-orbit (SO) energy, Δ_0 decreases with increasing tensile strain at the Γ -point. Also, the E_1 SO energy, Δ_1 at the Λ -direction remains constant indicating a very low shear deformation-related shift in the band structure. This added knowledge about the optical and dielectric constants of Ge thin films as a function of tensile strain can enable better design of Ge-based optoelectronics.

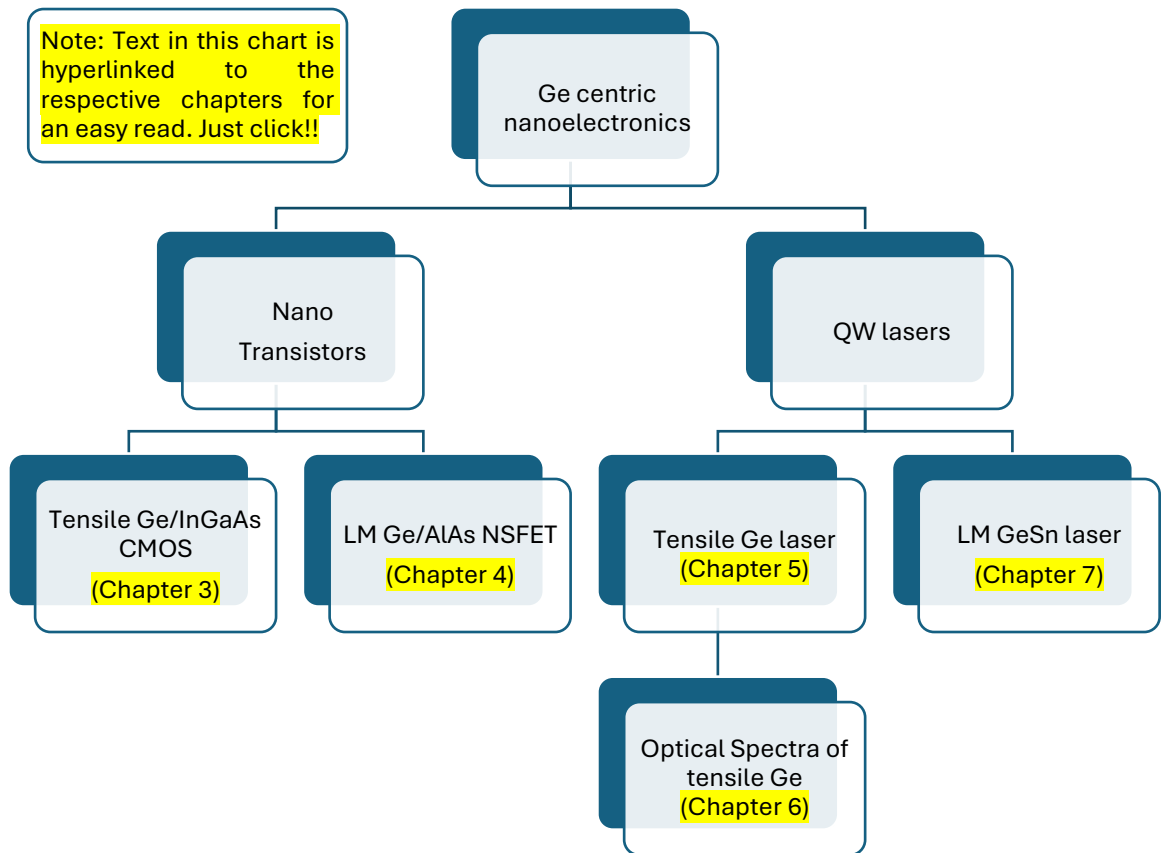
Tensile strain has interesting implications for Ge lasers, but, using tensile strain in the active region can be challenging in terms of reliability and mass manufacturing. This is due to the surface roughness, unwanted relaxation of strain, and associated defects. It may be desirable to avoid strain in a lasing system. A novel solution is discussed in this work through an introduction of a new lattice-matched lasing system, GeSn-InGaAs-InAlAs which has the potential to offer advantages of the GaAs-AlAs system discussed earlier and more. This work analyzes the use of $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ compositionally controlled epitaxial layers to form a SCH QW structure for the GeSn active layer, thus forming a complete laser structure. The key merit of this design is that the complete QW laser stack (GeSn QW, InGaAs waveguide, and barrier, InAlAs SCH layer, and contact layers) are lattice matched, resulting in no lattice-mismatched induced defects and potentially superior as well as reliable lasing performance. Additionally, the $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ layers can provide large band offsets with the GeSn layer to form a type I system with operability at room temperature. Furthermore, the lack of defects at the interfaces can mitigate any defect-induced band alignment changes away from type I. This InAlAs/InGaAs/GeSn/InGaAs/InAlAs SCH laser structure can achieve an excellent J_{TH} approaching $\sim 10 \text{ A/cm}^2$ at an emission wavelength of $\sim 2.6 \mu\text{m}$ while providing good net modal gain for a single QW configuration of $\sim 40 \text{ cm}^{-1}$. As a consequence of Sn composition-dependent

lasing wavelength, effective mass, band gap, and conductivity of the stack, the proposed GeSn laser can perform optimally for Sn compositions between 8 - 18 %.

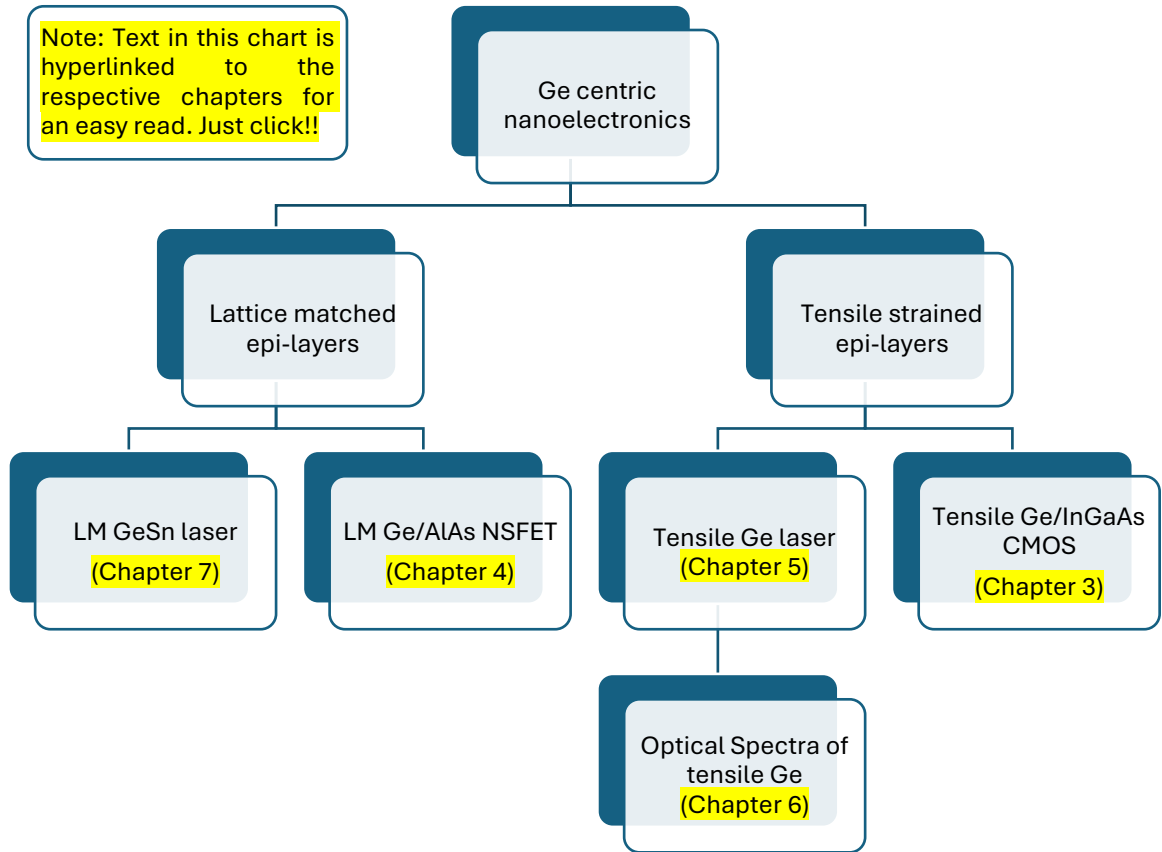
This LM GeSn QW SCH laser shows the potential to be an efficient, reliable, and tunable (1.2 μm to 6 μm wavelength) room-temperature light source, which can be monolithically integrated on a GaAs or Si substrate. The wide range of tunability of this GeSn QW laser as a function of Sn alloy composition and GeSn QW thickness will prove to be beneficial for a wide range of applications. The details of the theoretical investigation of the lattice-matched GeSn SCH QW laser are discussed in **Chapter 7**.

1.5 Dissertation Objective and Organization

The objective of this dissertation is to explore, analyze, and discuss two important applications of Ge epitaxial thin films in advanced electronics and photonics: *high-performance nanoscale transistors* and *efficient quantum well light sources*. Lattice matching as well as tensile strain gives rise to unique benefits and design considerations for both the categories of devices. So based on the type of Ge epi-layer growth leveraged for the active region, i.e., pseudomorphic (tensile strained) or metamorphic (lattice matched) the dissertation is sub-divided into the following chapters.



The chart presented above highlights the organization of this dissertation from a Ge device-application perspective: Nano transistors and QW lasers. Based on the type of epitaxial layers used in the device applications, a division is possible based on the type of Ge MBE growth: Lattice matched and Tensile strained, as shown in the classification in the chart below.



Chapter 1 introduces and motivates the idea behind exploring Ge-based nanoscale transistors for beyond the roadmap applications as well as Ge(Sn) based tensile and lattice-matched quantum well lasers for advanced photonics. **Chapter 2** explains the experimental, theoretical, and simulation techniques and tools used during this dissertation and the associated research efforts. It delves into the fundamentals of MBE growth of lattice-matched and tensile strained Ge systems, central to this study. Epitaxial thin films are grown using MBE and their composition and lattice structure are ascertained using X-ray diffraction spectroscopy (XRD), and a brief discussion is provided for the same. Further, the optical properties, dielectric spectra as well as band properties of epitaxial Ge thin films can be determined using variable-angle spectroscopic ellipsometry (VASE). The measurement, calibration, modeling, data processing, and interpretation of VASE for tensile strained Ge epitaxial thin films are discussed. Lastly, it highlights the methodology employed for simulation of the transistor and laser devices used in this dissertation using Sentaurus TCAD.

Chapter 3 motivates the need for a monolithic alternate channel tensile-Ge and InGaAs-based cointegrated CMOS as well as the structure, design considerations, performance metrics,

and trade-offs. A methodology to co-optimize the material, device, and circuit metrics and constraints is presented. Performance is evaluated at the advanced N5 FinFET node for the two complementary devices for 0.5V operation. **Chapter 4** scales this technology further to the advanced GAA nodes beyond N5 up to the Angstrom era. A complete Ge-based CMOS is envisioned and discussed in the context of process development, structure fabrication, performance, and challenges. The advantages of using a sacrificial lattice-matched AlAs layer are discussed. Using calibrated solvers, the device as well as inverter and SRAM circuit performance for this lattice-matched Ge-on-AlAs CMOS is presented.

Chapter 5 moves to photonic device technology based on epitaxial tensile strained Ge active layers grown on an InGaAs strain template. It discusses the fundamentals of semiconductor lasing, quantum well fundamentals, and other explorations of Ge lasers in literature. Finally, motivates the need for a tensile strained Ge-based quantum well light source on an InGaAs strain template, performance metrics, advantages, and challenges.

Chapter 6 delves deeper into the optical properties of tensile strained Ge epitaxial films. Using VASE, the dielectric spectra for tensile Ge are measured, and band artifacts associated with Van-Hove singularities are uncovered. This knowledge of the dielectric properties of epitaxial Ge and the impact of tensile strain provides better feedback for future design projects, as well as better understating and verification of the calculated k.p band structure of tensile Ge.

Chapter 7 introduces a new Ge system that can be lattice matched to the underlying layer either the InGaAs or InAlAs layer. This is the GeSn active layer lasing material that can achieve a direct bandgap without the use of tensile strain enabling superior material quality, and minority carrier lifetime. The lasing metrics such as threshold current, gain, loss, and IQE are presented here.

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Chapter 2 – Materials, Methods and Simulation Framework

2.1 MBE growth for the Ge-on-III-V material system

This work utilizes in-house MBE grown epitaxial structures involving Ge, GeSn and III-V compounds. These structures epitaxially grown using solid-source MBE, which is a thin-film deposition method. This section briefly describes the MBE growth methodology. MBE is a non-equilibrium growth process wherein, for a range of growth temperatures, epitaxy occurs by way of a mass transport-limited mechanism. The MBE growth conditions are such that the thermal evaporation or sublimation of high-purity, elemental sources produces a molecular beam of neutral atoms or molecules that is directed towards a growth substrate. In order to maximize the flux of material impinging on the growth surface, maintain a consistent growth environment, and minimize background contaminate incorporation during epitaxy, the growth chamber is kept under ultra-high vacuum (UHV), typically within the range of 10^{-10} Torr. This enables the mean-free path of the constituent atomic or molecular species to be large, thereby minimizing collisions between beam particles and residual gaseous species and promoting high-purity, low-defect epitaxy. Moreover, for the range of growth temperatures in which mass transport-limited growth is dominant, the cation beam flux (*e.g.*, gallium, Ga) determines the growth rate. As such, the growth rates in conventional MBE do not generally exceed several micrometers per hour ($\mu\text{m/hr}$), corresponding to a reduced elemental flux as compared to growth techniques employing alternative elemental sources, such as metalorganic chemical vapor deposition (MOCVD). However, the lower growth rates used in MBE offer a distinct advantage in that they offer the ability to engineer epilayer interfaces with near atomic precision [1-3].

The three primary modes of thin-film growth observed during epitaxy: (i) Frank-van der Merwe; (ii) Stranski-Krastanov; and (iii), Volmer-Weber [1-3]. In Frank-van der Merwe (F-M) growth, adatoms adhere to surface sites due to the weaker adatom cohesive force as compared to the surface adhesion force they experience. This results in 2D layer-wise epitaxy, which aids in preserving the crystallinity of the growing film. As film growth continues, the surface energy at the growth front is reduced, ensuring complete wetting of the surface and forming atomically smooth epilayers. Conversely, Stranski-Krastanov (S-K) growth marks a transition between growth modes, wherein epitaxy initially follows the F-M mechanism of growth until sufficient strain energy accumulates within the growing epilayer so as to modify the surface energy. At this

stage, the surface adhesion force becomes weaker than the adatom cohesive force, resulting in the nucleation of “islands” of material at the growth front, also known as three-dimensional epitaxy. Epitaxy that either initiates or continues (from a preceding growth mechanism) in a three-dimensional manner is known as Volmer-Weber (V-W) growth.

The MBE heterostructure growth consists of isolated III-V and Ge growth chambers connected via a UHV transfer chamber (base pressure $\sim 10^{-10}$ Torr). Isolation of the two growth chambers minimizes the chances of cross-contamination between group IV and III-V atomic species, and aids in limiting atomic interdiffusion at the Ge/III-V heterointerface[3-5]. Prior to being transferred into the III-V reactor, the epi-ready growth substrate (either (001)GaAs or (001)Si offcut 2° , 4° , or 6° toward a $\langle 110 \rangle$ direction) undergoes two successive outgassing procedures, the first occurring at 180°C for 120 minutes within a load-lock (base pressure $\sim 10^{-8}$ Torr), and the second occurring at 400°C for 60 minutes within the UHV transfer chamber. Outgassing of the growth substrate prior to introduction into the growth reactor reduces the potential for surface contaminants (e.g., volatile hydrocarbons) to be introduced into the growth reactor during oxide desorption, thus preserving thin film purity during epitaxy. Prior to growth of the Ge/III-V heterostructure, the substrate is desorbed of residual native oxides at either 750°C (GaAs) or 930°C (Si). For native Ga and As oxide desorption, an As_2 overpressure of $\sim 1 \times 10^{-5}$ Torr is utilized in order to avoid excessive volatilization of As from the GaAs substrate, which would otherwise result in a non-stoichiometric, Ga-rich growth surface that inhibits coherent epitaxy. Conversely, no As_2 overpressure is used when desorbing a Si substrate of native Si oxides.

Following oxide desorption, a GaAs epilayer is grown, which serves as either a homoepitaxial buffer (on GaAs) or a metamorphic buffer (on Si). For the $0.25\ \mu\text{m}$ homoepitaxial GaAs buffer grown on (001)GaAs substrates, a nominal growth rate of $0.5\ \mu\text{m/hr}$ and growth temperature of 650°C are used. We note that all temperatures discussed in this work refer to the thermocouple temperature as remotely monitored via calibrated Eurotherm 2404/8 PID controllers. For heteroepitaxial GaAs metamorphically grown on (001)Si, a more rigorous procedure is required to minimize anti-phase domain boundary (APB) formation during III-V growth (a well-understood consequence of polar on non-polar epitaxy) [6, 7] as well as reduce the total threading dislocation density stemming from the high degree of lattice mismatch between GaAs and Si ($f \sim 4\%$)[8, 9]. In brief, a combination of low growth rate ($\sim 0.09\ \mu\text{m/hr}$), low growth temperature ($\leq 400^\circ\text{C}$) epitaxy followed by successive high growth rate ($0.5\ \mu\text{m/hr}$), high growth

temperature ($> 400^{\circ}\text{C}$) epitaxy and annealing stages accomplishes the aforementioned objectives. With respect to the former, a 60 s pre-growth As surface saturation, followed by a short-duration low growth rate GaAs nucleation phase, inhibits APB formation when coupled with the slight substrate offset mentioned earlier. With respect to the later, the cyclical thermal annealing performed during the final stages of metamorphic buffer growth promotes the lateral glide and annihilation of threading dislocations, thereby limiting their propagation in the growth direction.

Growth of the AlAs high bandgap buffer or $\text{In}_x\text{Ga}_{1-x}\text{As}$ linearly graded buffer (LGB) proceeds immediately following GaAs buffer growth. Ge/AlAs epi-layers are leveraged for NSFETs in Chapter 4 whereas the tensile strained Ge/InGaAs epilayers are leveraged for alternate channel CMOS in Chapter 3 and for tensile Ge QW laser in Chapter 5 as well as for optical spectrum characterization in Chapter 6. A nominal growth temperature of 550°C is used for all $\text{In}_x\text{Ga}_{1-x}\text{As}$ LGB and constant-composition growths, irrespective of substrate type. On the contrary, due to the increased thermal conductivity of Si as compared to GaAs, and the low adatom surface mobility of Al, a reduction in growth temperature from 650°C to 600°C is necessary when growing AlAs on Si versus GaAs. An additional consequence of the low adatom surface mobility of Al is increased epilayer surface roughness, which can be partially mitigated by a reduction in the AlAs growth rate. The AlAs growth rate used in this work is $0.17\text{ }\mu\text{m/hr}$. The strain grading rate (the degree of misfit accommodated by the total LGB thickness) can be optimized so as to simultaneously inhibit threading dislocation propagation as well as maximize strain relaxation within the graded buffer [10, 11]. For the heterostructures investigated here, a general reduction in strain grading rate was observed for increasing In alloy compositions, thereby aiding in relaxation of the higher In alloy composition graded buffers and constant-composition stressors.

Upon completion of the III-V metamorphic buffer growth, the substrate is cooled to 150°C under an As_2 overpressure and subsequently transferred to the Ge growth reactor via the UHV transfer chamber discussed earlier. A low Ge growth temperature of 400°C , and growth rate of $\sim 0.065\text{ }\text{\AA}/\text{s}$, is used in order to minimize surface roughness and limit cross-species contamination during Ge nucleation and throughout the Ge epilayer growth [5, 6]. Lastly, we note that in-situ reflection high-energy electron diffraction (RHEED) analysis is used to monitor surface reconstruction at all stages of oxide desorption and growth, thereby providing real-time feedback regarding surface stoichiometry (i.e., Ga- or As-rich) and growth mode (i.e., two- or three-dimensional epitaxy). RHEED is an in-situ surface analysis technique that uses a high-energy

electron beam at an extremely shallow incidence angle in order to generate electron diffraction patterns corresponding to the top several monolayers of the material. The high electron energies used in RHEED (e.g., 14.3 kV and 1.43 A used in this work) result in a large-diameter Ewald sphere in reciprocal space, thereby capturing a similarly large number of reflections. The corresponding electron diffraction pattern (as observed via a phosphorescent screen) is thereby indicative of the growth mode of the thin-film. Under two-dimensional (F-M) epitaxy, the RHEED pattern consists of narrow, elongated diffraction points consistent with rows of orthogonal, intersecting atomic planes at the growth front's terminating surface. Deviation away from these growth conditions is reflected by a loss of diffraction point intensity and a disruption to the RHEED pattern's regularity, indicating a transition in the epitaxy mechanism (i.e., S-K or V-M growth).

The growth of GeSn-on-III-V growth proceeds as follows. Epitaxial $\text{Ge}_{1-y}\text{Sn}_y$ layers with varying Sn compositions from 0% to 6% were grown on semi-insulating (100)GaAs substrates that were 2° off towards $\langle 110 \rangle$ direction (with or without an intermediate AlAs buffer layer) using an ultra-high vacuum interconnected, dual-chamber MBE system with separate reactors for group IV and group III-V materials. The interconnected growth chambers minimize the atomic interdiffusion at the Ge/AlAs and strained Ge/InAlAs heterointerfaces. GeSn with 6% Sn composition was grown on graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffers starting from GaAs substrate. 7N highpurity Ge (American GMG Incorporated, United Mineral and Chemical Corporation) and 6N high-purity Sn (American GMG Incorporated) elemental source materials were used for this work. An in-situ reflection high energy electron diffraction (RHEED) module connected to the III-V reactor was used to monitor the GaAs substrate oxide desorption process, and the surface reconstruction of the III-V epilayers (i.e., GaAs, AlAs, and graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer) during growth. Likewise, the surface reconstruction of the as-grown Ge and $\text{Ge}_{1-y}\text{Sn}_y$ films were investigated following $\text{Ge}_{1-y}\text{Sn}_y$ epitaxy and transfer of the sample(s) from the group IV reactor to the group III-V reactor. This in-situ growth and analysis capability permitted the examination of the surface reconstruction for representative GaAs, Ge and $\text{Ge}_{0.97}\text{Sn}_{0.03}$ samples. The GaAs substrate oxide desorption was performed at 750°C under an arsenic flux of $\sim 10^{-5}$ Torr prior to reducing the temperature to 650°C for GaAs homoepitaxy. The temperature referred to herein was the thermocouple temperature. After the growth of the 250 nm GaAs homoepitaxial buffer, different thicknesses of AlAs were grown at 650°C prior to $\text{Ge}_{1-y}\text{Sn}_y$ epilayer growth. The 750 nm thick linearly graded $\text{In}_x\text{Al}_{1-x}\text{As}$ metamorphic buffer was grown at 480°C in order to balance the different adatom mobilities of

aluminum (Al) and indium (In) on the growth surface. The overshoot In composition of $\sim 16\%$ was incorporated within the graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer ($x \rightarrow 0.03-0.16 \rightarrow 0.12$) for efficient strain relaxation. After the graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer growth, a 15 minute, 580°C annealing step was implemented under an arsenic flux of $\sim 10^{-5}$ torr to provide thermal energy for annihilation of lattice mismatch induced defects. After annealing the graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer layer, a constant composition of $0.5\ \mu\text{m}$ thick $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ layer was grown at 580°C , which is lattice-matched to a $\text{Ge}_{0.94}\text{Sn}_{0.06}$ epilayer. The importance of lattice matching GeSn epi-layers is discussed QW laser applications in Chapter 7. Each layer structure was cooled down below 200°C under a decreasing As_2 overpressure, and vacuum ($\sim 4 \times 10^{-10}$ Torr) transferred to the group IV reactor for $\text{Ge}_{1-y}\text{Sn}_y$ epitaxy in the temperature ranges from 175°C to 250°C . The growth rate of the Ge film was calibrated to $0.1\ \text{\AA/s}$. The Sn cell temperature was varied for different Sn compositions. After the growth of each $\text{Ge}_{1-y}\text{Sn}_y$ film with different thicknesses and Sn compositions, each sample was cooled down to 50°C at a ramp rate of 5°C/min prior to unloading from the group IV reactor in order to prevent the formation of defects due to the dissimilar thermal expansion coefficients between each layers studied here.

Lastly, as many of the growths involve tensile strained samples, a note regarding critical layer thickness is provided here. During pseudomorphic or lattice mis-matched growth, a consideration regarding the epi-layer thickness arises which is not a concern during lattice matched growth. Accumulation of strain energy within the growing epilayer results in a distortion of the surface energy at the growth front, thereby instigating a transition from two-dimensional to three-dimensional epitaxy. This transition corresponds to an epitaxial film thickness, h_c , also known as the critical layer thickness, past which it is reasonable to expect both an increasingly irregular surface as well as an increasing number of crystalline defects within the epilayer. These structural defects are the result of relaxation processes occurring within the epilayer in order to relieve the accumulated strain energy. The dependence of h_c on the epilayer-substrate lattice constant mismatch (and hence strain energy present in the epilayer), commonly known as the misfit, f is popularly modeled with two models, Matthews and Blakeslee force balance model [12], and the People and Bean energy balance model[13].

2.2 XRD Characterization: Lattice matched and Mis-matched epitaxy

HR-XRD is an essential analysis technique used in the structural characterization and determination of strain relaxation properties in heteroepitaxial thin-films grown using MBE. The composition and strain for tensile Ge and GeSn (Chapter 3-7) on III-V are determined using similar XRD analysis. Basic structural analysis of XRD data utilizes the real and reciprocal space geometric equivalences for angular diffraction, *i.e.*, the Bragg and Laue equations, respectively, as given by

$$2d \sin(\theta_B) = n\lambda \quad (2.2.1),$$

where n is the order of reflection, θ_B is the Bragg angle, d is the inter-atomic plane spacing, and λ is the x-ray wavelength (1.540597 Å for XRD measurements). The corresponding Laue equation for reciprocal space can be written as

$$(hkl) = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (2.2.2),$$

where a is the crystal lattice spacing and (hkl) defines the indices of the atomic plane (in reciprocal space) being probed. Equating the two, the Bragg angle for a given atomic plane as specified by its (hkl) indices, $\theta_B(hkl)$, can thus be expressed as [14]:

$$\theta_B(hkl) = \sin^{-1} \left(\frac{\sqrt{h^2 + k^2 + l^2}}{2a} \right) \quad (2.2.3).$$

A more methodical strain relaxation analysis procedure applicable to the semiconductor heterostructures investigated herein requires the recording of x-ray reciprocal space maps (RSMs). RSMs consist of a large number (several hundred to several thousand) of ω -2 θ spectra (colloquially known as x-ray rocking curves) taken at incrementally different ω scan-center points, thus generating a two-dimensional map of angular diffraction intensity for a given sample, *i.e.*, a diffraction intensity contour plot. From the reciprocal lattice point (RLP) corresponding to the thin film(s) present in the sample, the ternary alloy composition (if applicable), lattice mismatch, and the strain relaxation properties of each epilayer can be determined. In order to do so requires the

recording of symmetric (004) and asymmetric (115) RSMs. Subsequently, the in-plane and out-of-plane lattice constants, $a_{\parallel}$ and $a_{\perp}$, respectively, for each epilayer can be determined utilizing the symmetric (004) and asymmetric (115) diffraction data and Bragg's law [14, 15]. The corresponding relaxed lattice constant, a_r , and epitaxial strain, ε , of each epilayer can then be found using,

$$a_r = \frac{2\nu}{1+\nu} a_{\parallel} + \frac{1-\nu}{1+\nu} a_{\perp}, \quad (2.2.4).$$

$$\varepsilon = \frac{a_r - a_s}{a_s} \quad (2.2.5).$$

where ν is the Poisson ratio of the epilayer and a_s is the bulk lattice constant of the substrate or virtual substrate (VS). We note this expression is only applicable to binary or ternary materials, *e.g.*, $\text{In}_x\text{Ga}_{1-x}\text{As}$, whereas elemental semiconductors, *e.g.*, Ge, need only consider $a_{\parallel}$ and the relaxed bulk lattice constant of the material, a_0 , when determining in-plane epitaxial strain, *i.e.*:

$$\varepsilon_{\parallel} = \frac{a_{\parallel} - a_0}{a_0}, \quad (2.2.6).$$

For ternary materials, ν can be estimated using Vegard's law and the elastic constants of the constituent binary materials, *e.g.*, GaAs and InAs. Moreover, due to the differing atomic species occupying the sublattices in binary and ternary materials, asymmetric strain relaxation can occur along the two orthogonal $[110]$ and $[1\bar{1}0]$ directions. As such, $a_{\parallel}$ could differ depending on the crystallographic orientation of the sample during XRD spectral recording. The corresponding relaxation as function of crystallographic orientation provides information regarding residual strain asymmetries within the binary or ternary epilayer, and can be expressed as [15, 16],

$$R_{[110]} = \frac{a_{\parallel,[110]} - a_s}{a_{\perp,[110]} - a_s} \text{ and } R_{[1\bar{1}0]} = \frac{a_{\parallel,[1\bar{1}0]} - a_s}{a_{\perp,[1\bar{1}0]} - a_s} \quad (2.2.7).$$

where $a_{\parallel,[hkl]}$ and $a_{\perp,[hkl]}$ are the epilayer's in-plane and out-of-plane lattice constants, respectively, as determined for the $[110]$ and $[1\bar{1}0]$ directions. In the case of isotropic strain relaxation, *i.e.*, $R_{[110]} = R_{[1\bar{1}0]}$, the average strain relaxation is given by,

$$R = \frac{R_{[110]} + R_{[1\bar{1}0]}}{2}, \quad (2.2.8).$$

The perpendicular lattice mismatch, $f_{\perp}$, for a binary or ternary epilayer with respect to an underlying substrate (or VS) can also be determined, and is given by,

$$f_{\perp} = \frac{a_{\perp} - a_s}{a_s}, \quad (2.2.9).$$

Similarly, the parallel lattice mismatch, $f_{\parallel}$, along each $[110]$ and $[1\bar{1}0]$ direction is given by:

$$f_{\parallel,[110]} = \frac{a_{[110]} - a_s}{a_s} \text{ and } f_{\parallel,[1\bar{1}0]} = \frac{a_{[1\bar{1}0]} - a_s}{a_s}, \quad (2.2.10).$$

Thus, for a fully relaxed binary or ternary epilayer, the lattice mismatch, f_r , can be written as:

$$f_r = \frac{1 - \nu}{1 + \nu} f_{\perp} + \frac{\nu}{1 + \nu} (f_{\parallel,[110]} + f_{\parallel,[1\bar{1}0]}), \quad (2.2.11).$$

Using these results, X-ray analysis was performed on selected samples to determine the Sn and strain composition as well as the overall structural quality of the layer using PANalytical X'Pert Pro X-ray unit equipped with pixel and proportional detector. As an example, the following discussion shows XRD analysis of LM 6% GeSn on InAlAs sample. **Figure 1(a) and (b)** show the recorded symmetric (004) and asymmetric (115) RSMs, respectively, from the $\text{Ge}_{0.94}\text{Sn}_{0.06}/\text{In}_{0.12}\text{Al}_{0.88}\text{As}/\text{In}_x\text{Al}_{1-x}\text{As}/\text{GaAs}$ structure, highlighting the RLP centroid for each epilayer. The Sn composition from the measured RSMs was found to be $\sim 6\%$. HR-XRD data reveal that the 350 nm thick $\text{Ge}_{0.94}\text{Sn}_{0.06}$ epilayer is indeed lattice matched with respect to the $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ virtual substrate (VS). As can be seen from the symmetric (004) RSM shown in

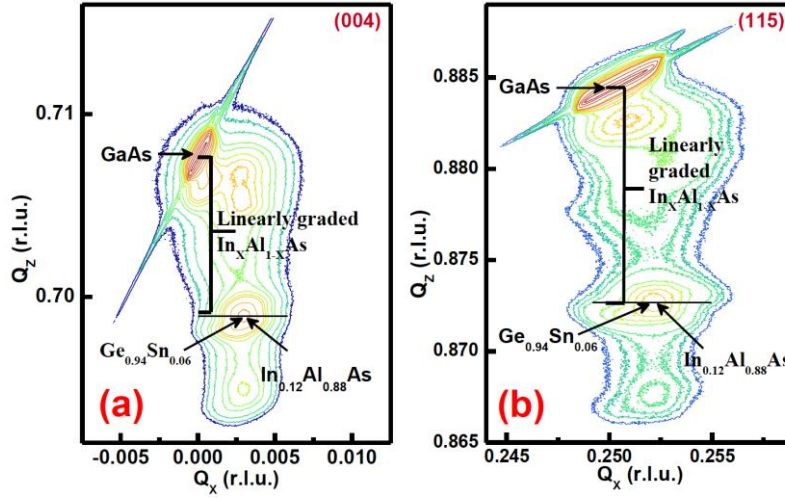


Figure 1. RSMs taken along the (a) (004) and (b) (115) orientations. These RSMs represent the lattice-matched epitaxy of 350 nm thick $\text{Ge}_{0.94}\text{Sn}_{0.06}$ on $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ buffer layer, which is expected to increase the carrier lifetime in GeSn layer due to reduced defects and improved material quality.

Figure 1(a), the in-plane lattice constant of $\text{Ge}_{0.94}\text{Sn}_{0.06}$ layer is matched with the upmost composition $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ of the graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer layer. **Figure 1(b)** further confirms the lattice-matched $\text{Ge}_{0.94}\text{Sn}_{0.06}/\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ heterostructure where the RLPs of both $\text{Ge}_{0.94}\text{Sn}_{0.06}$ and $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ layers are on top of each other. The overshoot In composition of 16 % embedded into linearly graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer (below the $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ RLP) is to relax the graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer layer. Further examination of (115) RSM (**Figure 1(a)**) reveals a close alignment in the Q_x components of the $\text{Ge}_{0.94}\text{Sn}_{0.06}$ and $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ RLPs, indicative of coherent lattice-matched epitaxy. Moreover, the Q_x - Q_z symmetry of the GeSn RLP suggests a uniform crystallinity absent of substantial mosaicity-inducing crystal defect scattering. Likewise, the narrow, symmetric nature of the $\text{In}_x\text{Al}_{1-x}\text{As}$ RLP indicates dislocation-minimal constant composition growth, signifying a strong confinement of mismatch-induced defects in the linearly graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer. Similar analysis was performed on a 50 nm-thick $\text{Ge}_{0.94}\text{Sn}_{0.06}$ epitaxial layer grown on GaAs with an intermediate 25 nm-thick Ge buffer, shown below.

2.3 Ellipsometric Optical Characterization (VASE): Tensile Ge

Ellipsometry is utilized to extract the optical and dielectric constants of the MBE grown tensile strained Ge samples. It is an optical characterization technique which is non-destructive and fast. It is a measurement sensitive to many bulk and surface properties as well as band structure dispersions. This sensitivity is obtained by measuring the phase change in the incident and reflected polarized light, thus making it immune to intensity changes. The VASE measurement yields two quantities, ψ and Δ values. These two quantities, ψ , and Δ , are related to the p- and s-polarization intensities through the relation [17, 18]:

$$\rho = \frac{R_p}{R_s} = \tan(\psi) e^{i\Delta} \quad (2.3.1)$$

where, ρ is the reflection coefficient ratio, R_p and R_s are the Fresnel Reflection coefficients [17,18]. The p-polarization is defined parallel to the incident plane and the s-polarization is perpendicular, thus forming an orthogonal coordinate system. For a single-layer structure like a smooth surface bulk substrate, ψ and Δ values can be directly converted to extract the refractive index (n) and extinction coefficient (k). As it can be seen, the measured quantity is a ratio, hence a great degree of accuracy and reproducibility can be achieved, often without the need for a reference sample. A

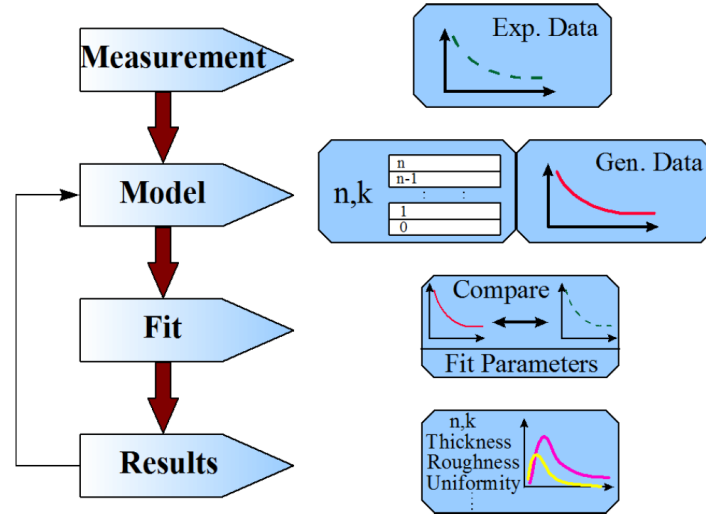


Figure 2. The measurement, modeling and fitting methodology for the VASE measurements using the J. A. Woollam VASE system [17, 18].

measurement, fitting and modeling algorithm for the VASE J. A. Woollam variable-angle-of-incidence spectroscopic ellipsometer system is adopted in this work and shown in **Figure 2**. More details of the methodology and measurement setup are provided in Ref. [17, 18].

The samples are mounted each onto the vertical stage of the J. A. Woollam variable-angle-of-incidence ellipsometer system [17]. The collection of data was performed for all the samples at room temperature and on the same day to avoid discrepancies due to changes in ambient and equipment configuration. The data was acquired over few angles of incidence such as 60°, 65°, 70°, and 75° chosen to be around the approximate Brewster's angle for material of interest, here Ge. A broadband Xenon lamp served as the light source, followed by a monochromator for wavelength selection. The incident light was polarized, and its polarization state was altered upon reflection from the sample surface. The reflected polarization was analyzed using a rotating analyzer and detected by a thermoelectrically cooled silicon/strained InGaAs stack photodiode detector. This process determined the ellipsometric angles ψ (amplitude ratio) and Δ (phase difference). The VASE measurement yielded ψ and Δ values with error bars of approximately $\pm 0.02^\circ$ and $\pm 0.06^\circ$, respectively. For the multilayer structures studied here direct extraction of the optical constants from raw data is not feasible. This is because ψ and Δ are coupled indicators of the optical properties of all the layers, including the surface conditions. An iterative process is necessary to decouple the contributions of each layer in the stack and determine their corresponding wavelength-dependent dielectric constants and thicknesses.

The objective of forming an accurate model is to decouple and extract the optical properties of Ge (n , k , ϵ_1 , ϵ_2 , and α) as a function of tensile strain from the measured values of ψ and Δ . The optical constants of InAs, GaAs, and $\text{In}_x\text{Ga}_{1-x}\text{As}$ are known as a function of wavelength and are available with the proprietary software suite WVASE provided with the J.A. Woollam VASE equipment [17]. The individual layer thicknesses and compositions of all the layers in the stack are known through precisely controlled MBE growth recipes calibrated with TEM and x-ray diffraction measurements. Due to the correlated nature of the optical constants and layer thicknesses, the thicknesses are held nearly constant around their nominal values during the regression analysis. This ensured that each best-fit thickness remained close to the global minimum of the mean squared error (MSE). The surface roughness and native oxide were effectively modeled as a single surface layer with its thickness as a free parameter. The index of this thin layer

was approximated using the effective medium approximation (EMA) to mix the indices of the Ge film and air in a 50:50 ratio [17, 18].

The optical constants for the epitaxial Ge layer were modeled using a Kramers-Kronig consistent General Oscillator (GenOsc) model. The GenOsc layer incorporates multiple parametric *Psemi* oscillators [19] corresponding to various regions of electronic transitions within the band structure measured in the spectra range of 0.5 eV to 4.1 eV.

2.4 Sentaurus TCAD simulation framework and methodology

In this section, a brief overview of these physical processes in a tensile strained Ge device as well as a composition dependent InGaAs device is discussed. First, a brief overview of the Sentaurus structure and device modeling is provided. 3D structures for the Ge and InGaAs FinFETs, multilayer Ge NSFETs as well as the Ge and GeSn QW laser are defined in the structure editor SDE. SDevice computes numerically the electrical behavior of a semiconductor device in or several physical devices combined using 3D interconnects or as spice elements in a circuit. Terminal currents, voltages, and charges are computed based on a set of physical device equations that describes the carrier distribution and conduction mechanisms. The 3D structure for the device under test is divided into meshing points, breaking down the computation into unit cells. The physical computations are performed on these unit mesh points and then interpolated. More details on the Sentaurus simulation flow are described in Ref. [20]. Various physical equations specific to the device are incorporated in the numerical solutions: drift-diffusion, multi-valley band structure, 6x6 k.p, piezo electric consideration of stress, band deformation, thermionic emission, recombination mechanisms, mobility effects, quantum density corrections, etc. More details on the Sentaurus device physics are described in Ref. [20]. The material and band parameters for various materials used are adopted from Ref. [20].

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Chapter 3 – Tensile Strained Ge and InGaAs Monolithic CMOS

3.1 Monolithic alternate channel CMOS: Material stack and FinFET device

Based on the tools and methods discussed in Chapter 2, a novel pathway for monolithic integration of Ge and InGaAs devices for high-speed electronics is presented in this section. This discussion explores the material system, simulation methodology, device performance considerations, and finally the CMOS circuit metrics for this cointegrated high mobility system. Currently, 4 methodologies are being pursued for the integration of high-performance Ge FinFETs: (i) Ge on insulator (Ge-OI) [1]; (ii) silicon-germanium (SiGe) graded buffer to bridge the lattice constant between the Ge and the Si [2]. The parallel conduction to the Ge channel created by the graded SiGe buffer is a limitation of such a structure and it can be avoided using a large-bandgap material like $\text{In}_x\text{Al}_{1-x}\text{As}$ or InGaAs. (iii) aspect ratio trapping (ART) to grow Ge on Si [3], and (iv) Ge on Si or GaAs using a III-V graded buffer. In the latter case, the growth of ε -Ge on $\text{In}_x\text{Ga}_{1-x}\text{As}$ or $\text{In}_x\text{Al}_{1-x}\text{As}$ can be achieved through a solid source molecular beam epitaxy (MBE) utilizing separate group III-V and group-Ge growth chambers, connected via an ultra-high vacuum transfer

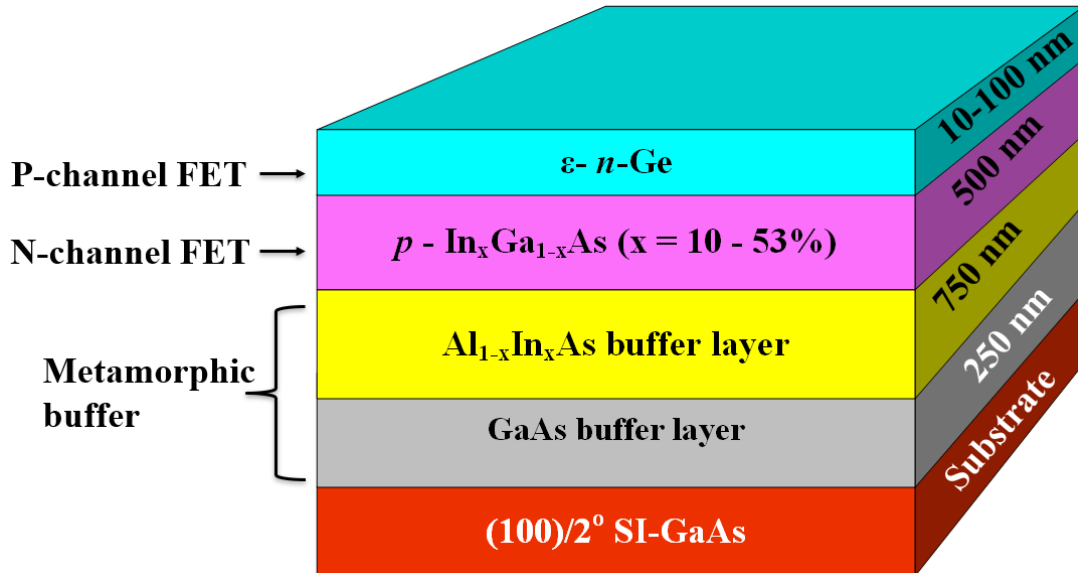


Figure 3. The InGaAs and Ge system on a lattice matched graded buffer grown on a semi-insulating GaAs substrate via InAlAs-GaAs buffer.

chamber [4,5]. Interestingly, utilizing the high bandgap III-V graded buffer methodology, the underlying layer can be InGaAs thus forming a high electron mobility channel for the n-channel device, thus putting a cointegrated hybrid CMOS system within reach. The ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ heterojunctions can be grown on a GaAs or Si substrate using either $\text{In}_x\text{Ga}_{1-x}\text{As}$ or $\text{In}_x\text{Al}_{1-x}\text{As}$ graded buffer, which will accommodate the lattice mismatch induced defects and dislocations, and the active layer will be virtually defect-free. The targeted In composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$ can be selected for a specific amount of tensile strain in Ge. Detailed growth and material characterization for the tunable ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ heterostructures using this MBE system is reported elsewhere [4,5] and also discussed in **Chapter 2**. A key benefit of Si-based CMOS is the monolithic nature of the growth and fabrication process which enables high-volume wafer fabrication. So, a search for alternate channel CMOS technologies must involve monolithic solutions that can offer additional advantages beyond Si. The monolithic system explored in this work is the tensile Ge on InGaAs hybrid system grown on a GaAs substrate through lattice grading buffers [4]. Such a growth on a GaAs substrate is further transferrable to a Silicon substrate for high-volume manufacturing using a thick lattice grading buffer [5]. Such a transferrable growth to Si remains the ultimate objective of most alternate channel device explorations. The epitaxial multi-layer structure is shown in **Figure 3**. The p-FinFET will be lithographically patterned in the upper tensile strained Ge layer utilizing the benefits of high mobility and low bandgap associated with this layer, thus enabling high-performance low power operation for the p-FinFET. The high electron mobility

n-FinFET is formed in the underlying InGaAs layer, thus enabling high performance and low power operation for the n-FinFET as well. The InGaAs layer and its In composition needs to be carefully chosen as it impacts the cumulative performance of this cointegrated CMOS system. A detailed study of this cumulative performance is summarized in this chapter. As the InGaAs layer houses the n-FinFET channel, its inherent doping should be intrinsic or p-type as shown in **Figure 3**. During MBE growth in our system, the InGaAs epi-growths typically have unintentional p-type doping of $5 \times 10^{17} \text{ cm}^{-3}$. Similarly, the tensile Ge top layer houses the p-FinFET channel, hence the n-type doping is unintentionally of the order of $\sim 2 \times 10^{18} \text{ cm}^{-3}$. The thickness of the uppermost constant composition layer of $\text{In}_x\text{Ga}_{1-x}\text{As}$ graded buffer (e.g., $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$) is large enough (e.g., 500 nm), hence providing a high degree of freedom in choosing the fin height of n-FinFET. On the contrary, the critical layer thickness for ϵ -Ge on $\text{In}_x\text{Ga}_{1-x}\text{As}$ becomes an important factor for such pseudomorphic growth limiting the possible fin height for the p-FinFET. High In composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$ (e.g., 53 %) shows a drastic reduction in the critical layer thickness of ϵ -Ge, limiting the fin height and creating a roadblock for achieving high fin aspect ratio. Utilizing the monolithic material stack shown in **Figure 3**, a cointegrated CMOS system can be formed, and a schematic representation of such a FinFET CMOS inverter configuration is shown here in **Figure 3**. This can be done by standard lithographic process steps sequentially. Here, the CMOS inverter is formed with n- and p-FinFET each having 3 fins for improved drive currents. The number of fins can be

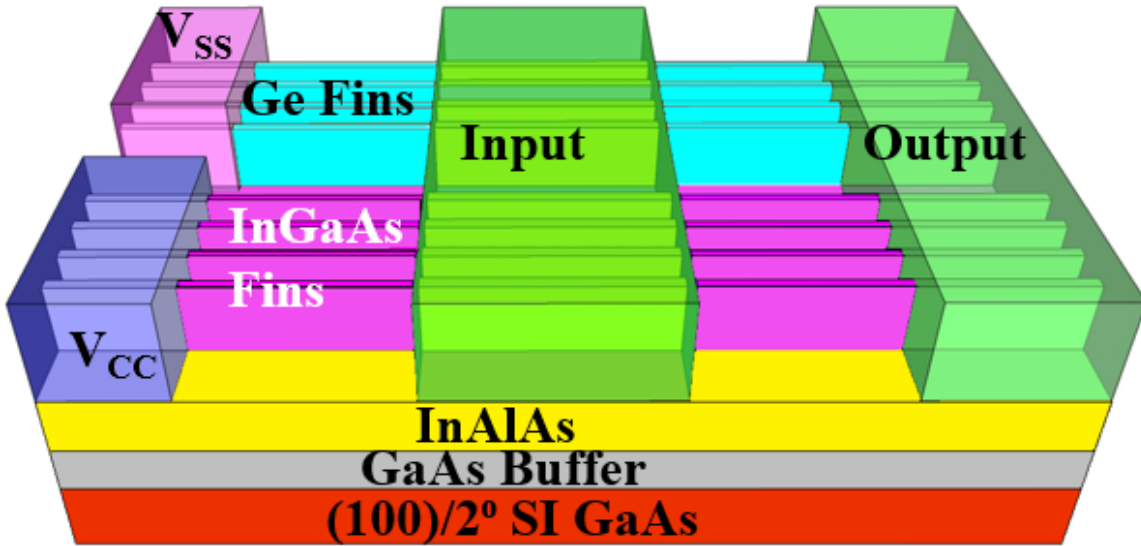


Figure 3. Cointegrated FinFET based CMOS utilizing $\text{In}_x\text{Ga}_{1-x}\text{As}$ n-channel and Ge p-channel for realizing an inverter

adjusted to enable current matching. The fabrication of such a CMOS structure will proceed by masking one device (say, the fabricated Ge p-FinFET) while the other is being processed, thus avoiding cross-contamination. While the Ge top device is fabricated and masked, the InGaAs active region is created by etching the Ge region over the active region. The In compositions in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer will affect the overall performance of this cointegrated CMOS in three significant ways: (a) the change in band structure due to increase in In composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$ leads to a lower bandgap and a higher mobility of electrons, (b) higher In results in increase in biaxial tensile strain in Ge layer, and (c) limits the critical layer thickness of $\epsilon\text{-Ge}$. The optimum choice of In composition and tensile strain can enable efficient CMOS operation, and the various design considerations to achieve this are discussed in the following sections.

3.2 Multi-physics model, strain-bandgap simulation, and model calibration

Understanding the various physical phenomena associated with the cointegrated CMOS system requires a multi-physics self-consistent solver that can capture many ideal and non-ideal phenomena, such as the Sentaurus-TCAD device simulator. Details about the Sentaurus multi-physics simulation of 3D devices were discussed in Chapter 2. A transistor is said to be operable for CMOS applications when the charges in the channel can be modulated considerably within the operating voltage range (here, $V_{GS} = V_{DS} = 0.5$ V). This implies that the transistor is normally-off, the V_{TH} lies within the supply voltage range, and the I_{ON}/I_{OFF} ratio is > 1000 [6]. The device performance can be characterized by SS and DIBL, which indicate the leakage and the V_{TH} change due to the effect of drain bias, respectively. The SS and DIBL should be as small as possible, where the SS can be as low as ~ 60 mV/dec at 300 K and DIBL can approach ~ 0 mV/V.

The simulations performed in Synopsys Sentaurus TCAD [7] using a 3-dimensional (3D) solver which considers the classical and quantum confinement effects within the fin structure as discussed earlier. To account for non-ideal interface properties and simulate realistic electrostatic properties of a FinFET, traps were incorporated at each critical heterointerface within the device structure. Trap states at the interfaces of each structure were modeled using a Gaussian distribution approximation. Electrons and holes distribution within the n-FinFET and p-FinFET devices were assumed to follow the Fermi-Dirac statistics. A 6-band $\mathbf{k}\cdot\mathbf{p}$ model was used to calculate the effective band structure as well as the mobility of electrons and holes in the presence of tensile strain in Ge. This was solved self-consistently with the Modified Local Density Approximation (MLDA) utility to account for quantum mechanical correction of the potential within the 3D-fin. The transport of carriers was computed using continuity equations considering the drift-diffusion physics [7], assuming a constant temperature profile across the device, which is a reasonable simplification in low-power logic devices.

Stress-induced change of the band structure of Ge requires the consideration of several valleys in the conduction band (CB) and the valence band (VB) to compute the correct dependency of the carrier concentration on the quasi-Fermi level. The computation of carrier densities and density of states (DOS) needs a multivalley solution approximation for the band-structure of the semiconductor. A fast computation of the Fermi integral of order $1/2$ ($F_{1/2}$) was performed using the Joyce-Dixon iterations. The number of Gauss-Laguerre integration points was restricted to 30 to

get an accurate result. A 6-band k·p band-structure was used to approximate the material band structure, with 4-bands for the VB and 2-bands for the CB within the Sentaurus device solver.

The tensile strain applied by the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer on the Ge channel is modeled using the Piezo-electric utility [7]. Computations of the change in the strain-induced band structure were performed based on the deformation potential theory [8]. The change in energy of each carrier valley or band, caused by the small deformation of the lattice, is a linear function of the strain. Stress to be considered here is the force per unit area applied on the face of the Ge lattice due to the difference in the lattice constants of Ge and $\text{In}_x\text{Ga}_{1-x}\text{As}$ for the Ge p-FinFET device. The Hooke's law for isotropic media,

$$\begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{bmatrix} = \frac{1}{E} \begin{bmatrix} 1 & -\nu & -\nu & 0 & 0 & 0 \\ -\nu & 1 & -\nu & 0 & 0 & 0 \\ -\nu & -\nu & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2+2\nu & 0 & 0 \\ 0 & 0 & 0 & 0 & 2+2\nu & 0 \\ 0 & 0 & 0 & 0 & 0 & 2+2\nu \end{bmatrix} \begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{bmatrix}, \quad (3.2.1),$$

where E is the Young's modulus for uniaxial stress, ν is the Poisson's ratio, σ is the stress tensor, and ε is the lattice mismatch tensor, is simplified for anisotropic cubic crystals considering their cubic symmetry [9]. The simplified compliance matrix of (Eq 3.2.1) for a cubic crystal can be solved for the case of a Zinc-Blende Ge lattice assuming a heteroepitaxial growth along the z direction and the growth plane parallel to the x - y plane. The growth of Ge on $\text{In}_x\text{Ga}_{1-x}\text{As}$ results in biaxial tensile strain on the Ge epitaxial layer. The in-plane stresses are equal, $\sigma_{xx} = \sigma_{yy} = \sigma_{||}$ for a cubic crystal, and the out-of-plane stress is assumed to be $\sigma_{zz} = 0$. The tetragonal lattice distortion can be represented in terms of the in-plane lattice constant, a , and the out-of-plane lattice constant, c . The in-plane and out-of-plane strains can be calculated using,

$$\varepsilon_{\text{in-plane}} = \varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{||} = \frac{a - a_0}{a_0}, \quad (3.2.2),$$

$$\varepsilon_{\text{out-of-plane}} = \varepsilon_{zz} = \frac{c - a_0}{a_0}, \quad (3.2.3),$$

where the in-plane and out-plane strains are related as $\varepsilon_{out-of-plane} = -R_B \varepsilon_{in-plane}$, where R_B is the biaxial relaxation constant and a_o is the substrate lattice constant. The elastic compliance constants (S_{ij}) along the 3 orthogonal directions can be calculated from the strain tensor:

$$S_{xx} = S_{yy} = \sigma_{||} = Y \varepsilon_{||} , \quad (3.2.4),$$

$$S_{zz} = -\sigma_{||} R_B = -Y R_B \varepsilon_{||} , \quad (3.2.5),$$

where Y is the Young's modulus for biaxial stress [9].

Pseudomorphic growth can result in either compressive or tensile strain on the epitaxial layer depending on the relative difference between the lattice constants of the substrate and the epitaxial layer. When the substrate lattice constant is smaller than the epitaxial layer (*e.g.* Ge on SiGe growth), the resultant epitaxial layer experiences positive in-plane stress ($\sigma_{xx} = \sigma_{yy} = \sigma_{||} = +ve$). This results in a biaxial compressive strain causing an upward shift in the Γ -valley with respect to the L-valley, resulting in an increase in the difference Δ . The degeneracy between the heavy hole (HH) and light hole (LH) bands is broken as a result of this compressive strain, and the HH band (holes with higher effective mass), moves upward. The Ge bandgap experiences a slight

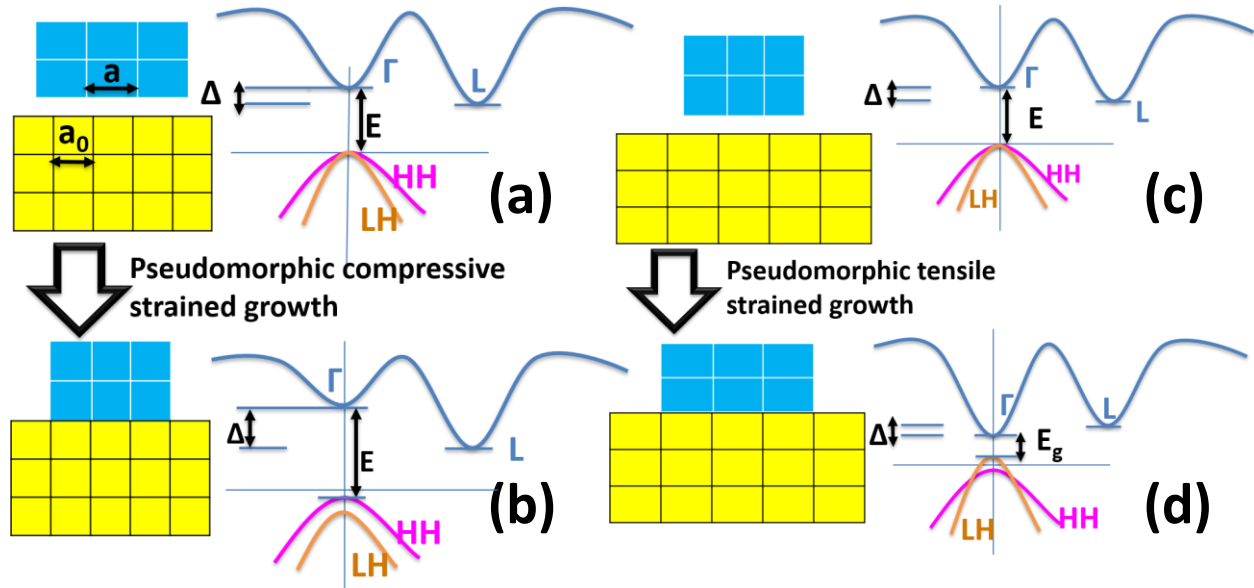


Figure 4. Schematic representation of pseudomorphic epitaxial growth and corresponding change in band structure: compressive strain $a_0 < a$ (a) before and (b) after growth. Tensile strain $a_0 > a$ (c) before and (d) after growth. Here, Δ is the separation between

increase due to the shift of HH and LH bands downward, and the band gap is determined by the minima of the L-valley and the maxima of the HH band as shown in **Figure 4(a) and (b)**.

Tensile strain is generated on the epitaxial layer when the lattice constant of the substrate is larger than the epitaxial layer, and the resultant in-plane stress is negative ($\sigma_{xx} = \sigma_{yy} = \sigma_{||} = -ve$). This results in a biaxial tensile strain as shown in **Figure 4(c) and (d)** causing a downward shift in the Γ -valley, resulting in a decrease in Δ . The degeneracy between the HH and LH bands is broken as a result of tensile strain, and the LH band (holes with lower effective mass), moves upward. For an In composition under 20 %, the tensile strain (< 1.5 %) is small and the bandgap is indirect [10]. Beyond 20 % In, Ge transitions to direct band-gap, and E_g is now determined by separation between the Γ -valley and the LH band, both of which are affected strongly by tensile strain. Thus, tensile strain results in a two-fold improvement in material properties of Ge (bandgap reduction and mobility boost) and hence, provides superior transistor performance. This work investigates the optimum region of operation while keeping the CMOS response symmetric, noise-immune, and power-efficient. The calibrated model for the tensile Ge p-FinFET [3] and InGaAs n-FinFET[11] based on experimental reports is shown in **Figure 5**.

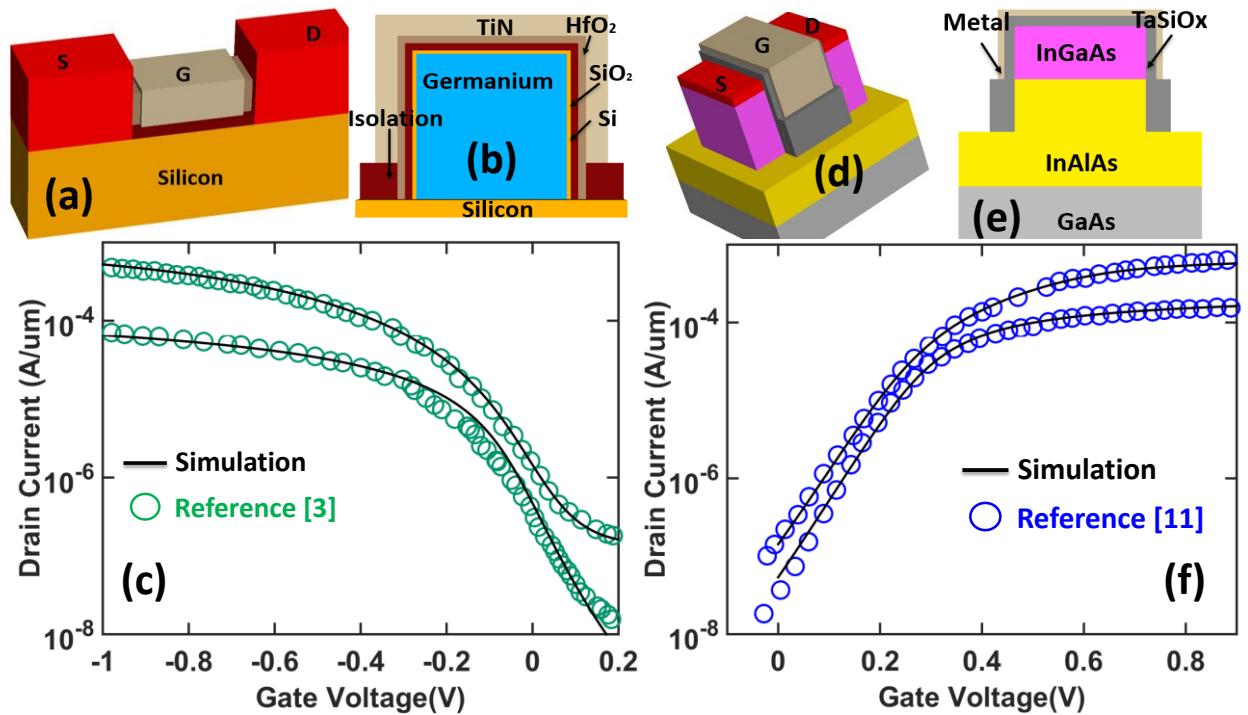


Figure 5. FinFET 3D structures and model calibration: Ge-on-Si p-FinFET (a) 3D structure, (b) gate stack, and (c) model calibration [3]. InGaAs n-FinFET (d) 3D structure, (e) gate stack, and (f) model calibration [11].

3.3 Device performance evaluation: Ge p-FinFET and InGaAs n-FinFET

Novel materials and device architectures, if aiming to improve upon existing Si-based transistors require considerations of the trade-off between the device/circuit performance and manufacture-feasibility. Further, a **material-device-circuit co-optimization** methodology is required to build the best possible *CMOS units* for the specific applications. After the previous discussion on the epitaxial material system for this monolithic Ge-on-InGaAs CMOS as well as the band and model calibration, a discussion on the device performance is warranted. The scaling of conventional Si complementary metal-oxide-semiconductor (CMOS) device feature size faces several technical device level challenges, including minimization of off-state leakage current (I_{OFF}); maintaining high drive current (I_{ON}) for circuit fan-out and high-speed operation; and supply voltage (V_{DD}) scaling to reduce total power dissipation and increase performance per watt while maintaining good noise margins. One must note that this scaling of device geometries comes through extensive R&D over years using very expensive lithography and process tools. Although scaling improves density, performance (on-current and drive strength), and profit per unit wafer, it is not an easy process. A potential way to alleviate this aggressive scaling requirement is to look for novel materials that can perform better than Silicon. The material properties researchers first look for are bandgap, electron and hole mobility, crystal growth know-how, and the ability to introduce active dopants. Ge and InGaAs are both uniquely positioned to provide all of these. At the device level, scaling the device length enables the electrons to travel faster from the source and drain resulting in shorter delays and faster device operation, *i.e.*, a large on-current. But, using Ge for the p-FinFET channel and InGaAs for the n-FinFET channel, we already have access to much larger electron mobilities, *i.e.*, an alternate way to get large on-current as opposed to just making the length smaller. Hence, this study will first explore how this novel CMOS cointegrated system performs in the moderately scaled length regime, *i.e.*, 60-110 nm. At this size, the lithography and process steps are relatively straightforward due to the Si-process know-how, and later an analysis and discussion will be presented at much advanced nodes up to the N0.7 node.

To leverage the performance benefits of having a high electron mobility n-channel InGaAs FinFET and high hole mobility p-channel Ge FinFET, this work explores a cointegrated alternate channel CMOS, as shown in **Figure 3**, whereas the ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ CMOS layer structure is shown in **Figure 3**. The variable In compositional $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer on graded $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer

will be used for the n-channel FinFET and the ε -Ge on top of this $\text{In}_x\text{Ga}_{1-x}\text{As}$ as a p-channel FinFET. This ε -Ge/InGaAs co-integrated system is studied in a FinFET gate architecture that provides excellent electrostatic control over the channel in comparison to conventional MOSFET, while being a manufacturable reliable architecture that has been in industrial production for almost a decade. The access to high electron and hole mobility channels enables the reduction of the power supply voltage down to 0.5V while maintaining good drive and noise margins.

Device characteristics such as V_T , I_{ON} , I_{OFF} , I_{ON}/I_{OFF} ratio, and SS are important parameters to assess the performance of nanoscale logic devices. These device parameters are analyzed at a supply voltage of $V_{CC} = 0.5 \text{ V}$ according to IRDS definitions [12]. The calibrated model discussed in the previous section is transferred onto the layer stack in **Figure 3** to realize the co-integrated CMOS structure. The channel doping of the n-FinFET and p-FinFET were adjusted ($N_A = 2 \times 10^{15} \text{ cm}^{-3}$ and $N_D = 4.8 \times 10^{18} \text{ cm}^{-3}$) to tune the region of operation (V_T) in the voltage range of 0 to 0.5 V, while ensuring that the V_T of the two devices are relatively close to each other in the range $0.10 \leq x \leq 0.53$. The device dimensions of the n-FinFET and p-FinFET are set at $L = 60 \text{ nm}$, $W = 40 \text{ nm}$, $H = 40 \text{ nm}$ to maintain the closest correlation between the experimental works reported for

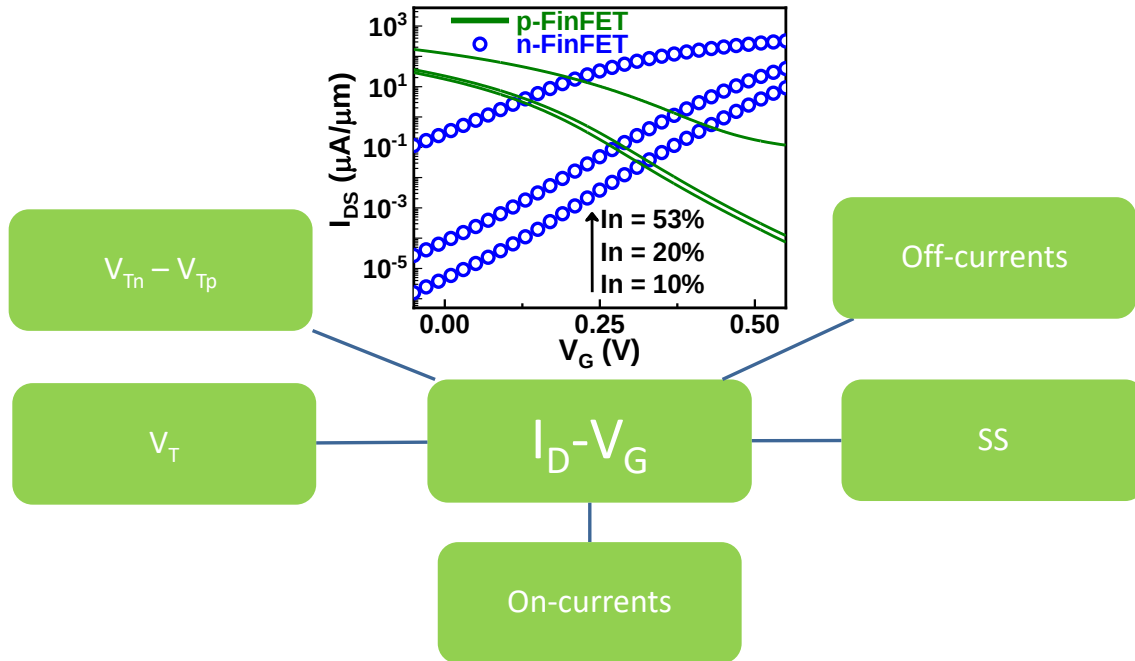


Figure 6. Drain current vs gate voltage ($I_{DS}-V_G$) characteristics for the tensile strained Ge p-FinFET and the InGaAs n-FinFET for a 1:1 fin ratio. The impact of the In % in the InGaAs layer is seen to affect the $I_{DS}-V_G$ significantly for both the devices. Various device metrics are extracted from the I_D-V_{GS} .

such material systems and the calibrated models [3, 11] discussed in the previous section. The advantages of scaling the process and the device parameters as well as the impact of short channel effects are explored in this section. The drain current I_{DS} vs gate voltage (V_G) for the tensile strained Ge p-FinFET and InGaAs n-FinFET shown in **Figure 6** indicates a shift in the relative operating regime for the two complementary FETs as a function of In composition. Various metrics such as on-current, off-current, SS, and V_T are extracted from the I_{DS} vs V_G to determine the quantitative impact of the In composition and tensile strain. Three representative In composition are shown in **Figure 6**, to illustrate the importance of choosing the optimum In composition to enable suitable CMOS operation. Owing to the complementary performance, one can notice that the InGaAs n-FinFET turns on at $V_G=0.5$ V demonstrated by the large current, whereas the tensile Ge p-FinFET turns off at this gate voltage indicated by the very small current. Throughout this quasi-stationary simulation, the gate voltage is ramped from 0 V to 0.5 V whereas the source voltage is kept fixed at 0V for the n-FinFET and 0.5V for the p-FinFET.

The first obvious change due to the In composition and the corresponding tensile strain is the change in the “turn-on point”, or the voltage at which the devices switch. This switching point is defined as the threshold voltage V_T and has many definitions, empirical and physics-based. Using the empirical definition based on the off-current value, the V_T of these two devices are equal at ~ 35 % In composition and diverge slightly above and below this value as shown in **Figure 7**,

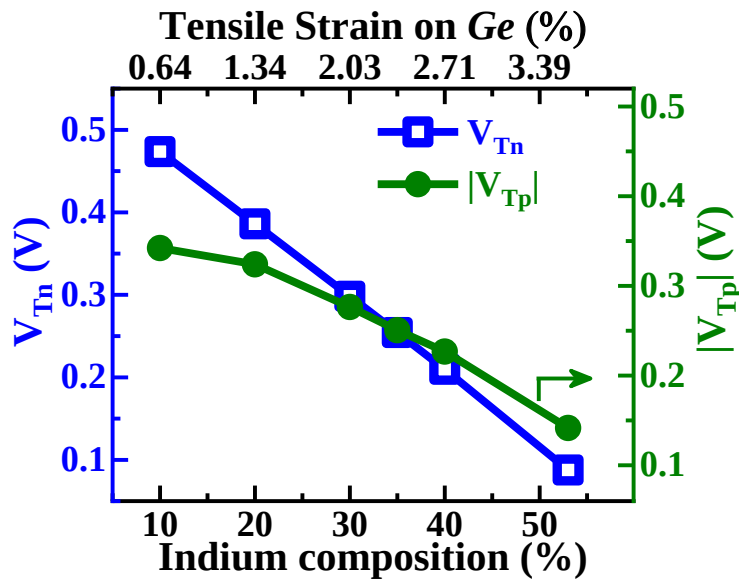


Figure 7. Threshold voltage of the two complementary devices, InGaAs n-FinFET and tensile Ge p-FinFET as a function of In % and corresponding tensile strain. A cross-over is seen.

this ensures CMOS functionality over this range of In compositions. The exact crossover point is a function of the chosen geometry, dimensions, gate dielectrics, doping etc. Detailed multi-parameter optimization is possible based on these independent parameters to determine better designs, but that is outside the scope of this study. From the structure, materials, models, and experimental references discussed in earlier sections, it is evident from **Figure 7** that the proposed cointegrated CMOS system can operate within the 0.5 V supply voltage, and the V_T for the two devices can be tuned to stay in this range for normally-off operation. Further, the V_T can be tuned for the two devices to obtain a matched complementary response. Increasing the In composition reduces the bandgap of the InGaAs channel for the n-FinFET thus resulting in a decreasing V_T . Consequently, increasing the In composition also increases the tensile strain as seen in the top x-axis scale in **Figure 7**. This results in a reduced bandgap for the Ge channel for the p-FinFET causing the V_T to reduce. A smaller channel bandgap indicates a smaller barrier for the electrons to cross from the source to the drain. A smaller barrier indicates a smaller threshold voltage at the gate.

The next important metric which is affected by the changing mobilities, bandgap and transport through the channels due to the increasing In composition, is the on-current (I_{ON}) shown in **Figure 8**. The impact of increasing the In composition is arguably the most important, and can be seen to have a monotonous increasing trend. Indicating that the on-current can be increased

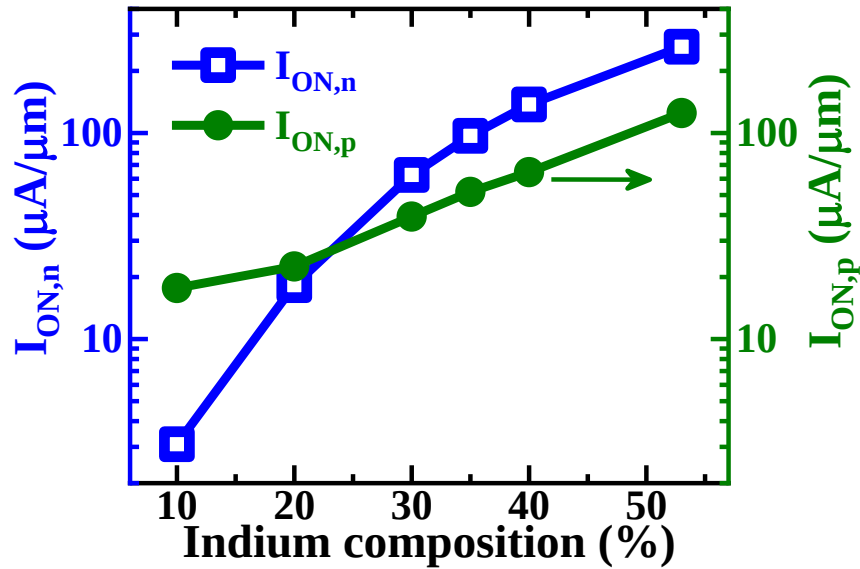


Figure 8. Impact of increasing the In composition and corresponding tensile strain on the on-currents of the two complementary devices.

significantly for both the devices by increasing the In composition and the corresponding tensile strain. This implies that for driving large fan-out loads and high speed operation, a larger In composition is beneficial for both the devices. For the tensile Ge p-FinFET, as the tensile strain is increased from 0 to 3.3% using the In composition, the on current is seen to increase by nearly 1 order of magnitude. Interestingly, the InGaAs n-FinFET sees an increase in on-current of more than 2 orders of magnitude. Again, a crossover point is seen for the two complementary devices at $\sim 20\%$. The objective of studying the on current is to determine the point where the n- and p- FETs can provide nearly equal current. However, the exact matching point will also be influenced by the V_T crossover seen earlier in **Figure 7**. The trend in **Figure 8**, can be understood using two physical mechanisms, tensile strain and alloying effect on bandgap and mobility. The increasing In composition in the InGaAs layer resulting in a decreasing bandgap for the n-channel while also increasing the mobility. A reducing bandgap means a smaller gate barrier and a larger current for a given supply voltage of 0.5 V. Additionally, a larger mobility of the electron carriers in the channel implies a larger on-current. So, for the case of the InGaAs n-FinFET, the increasing In composition results in a two-fold increase in the on-current, thus explaining the much larger change in the device on-current compared to the p-FinFET seen in **Figure 8**. Increasing the In composition also increases the tensile strain experienced by the Ge epi-layer housing the Ge p-FinFET. The on current for the Ge p-FinFET also increases due to the reducing bandgap due to

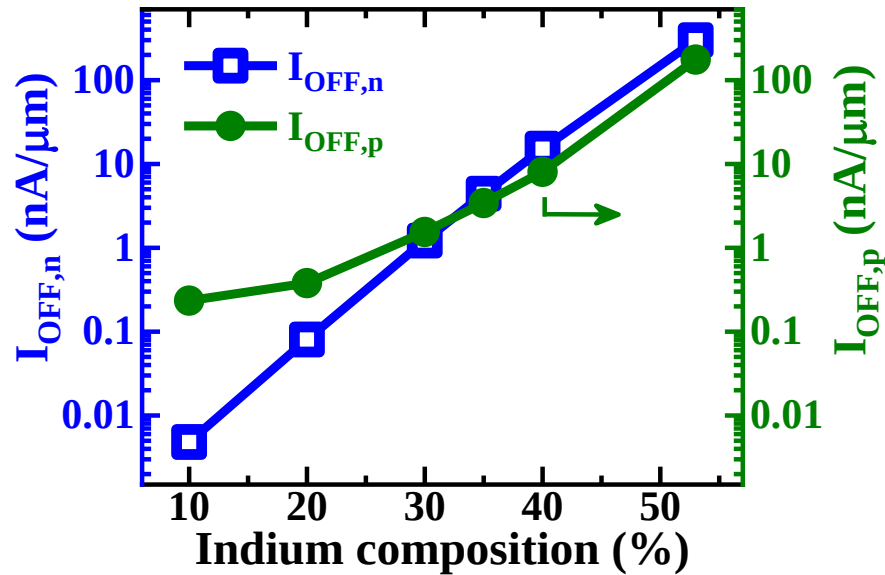


Figure 9. Impact of the In composition on the off-current for the tensile strained Ge p-FinFET and InGaAs n-FinFET.

the tensile strain, as well as the hole mobility enhancement associated with the LH-band movement. The impact of the hole mobility enhancement is relatively less pronounced due to the low DOS of the LH band, hence the total on-current enhancement due to the tensile strain is large but not as large as the InGaAs enhancement.

Leakage for the two devices off-state is another important metric as the number of transistors on a die approaches billions. This means that a leakage value of even 1 pA per transistor on the die can cause a total power dissipation of the order of ~ 1 mW. This implies an excessive drain on the battery power and increased total power consumption even when the component is turned off. Note that the total power consumption during high-frequency switching in the active state is much higher than this. The leakage for the Ge p-FinFET and InGaAs n-FinFET can be quantified as the off-current seen in **Figure 9**. Although a cross-over point is visible here too, it is of little significance as the objective is not to match the off-currents, but to reduce both as much as possible. But, a trade-off effect is seen to happen here, increasing the In composition is increasing the off-current, just like the increase in on-current seen earlier. This makes sense, as a reduced bandgap and increased mobility will improve the overall conductivity of the channel, resulting in more on-current as well as more off-current. So, the benefit of increasing the tensile strain and In composition seen in **Figure 8** needs to be balanced with a large associated increase in off-current. The roughly 4 orders of magnitude rise in off-current is a serious concern, thus

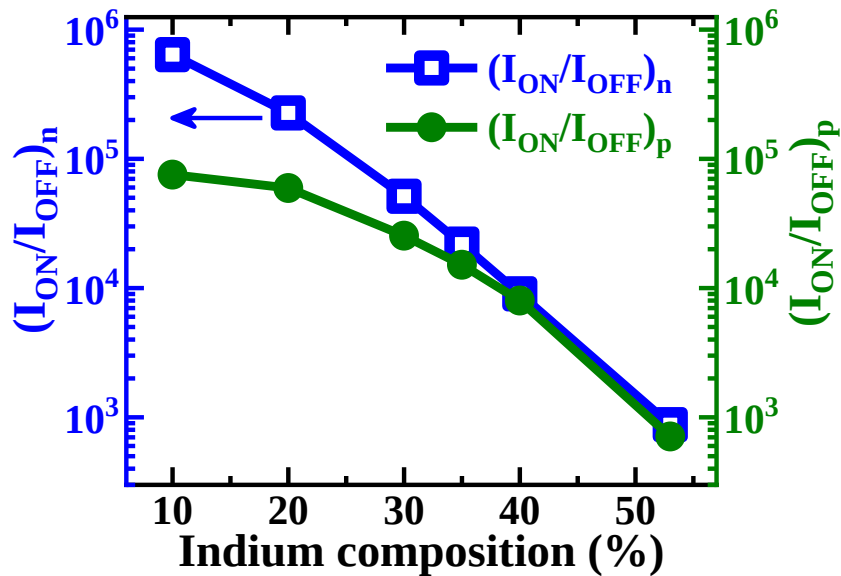


Figure 10. The ratio of the on-current to the off-current to determine a balance between the two, as a function of In composition.

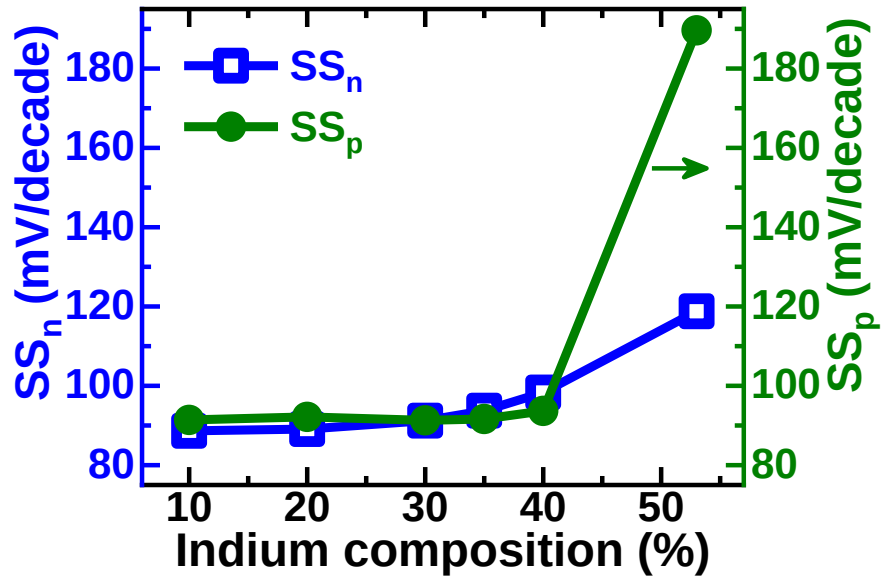


Figure 11. Impact of the In composition and tensile strain on the SS for the Ge p-FinFET and InGaAs n-FinFET

warranting an upper limit on the In composition. The In composition affects the on-current and the off-current, making the former better and the latter worse. Hence, it makes sense to define a ratio, to determine the best possible value of the In composition while balancing both. This ratio of on-current to off-current is shown in **Figure 10**, and a clear dominance of the off-current trend is seen in determining the on-off ratio. It is evident that the on-off ratio gets worse with increasing In composition, just like the off-current trend. The on-off ratio determines the difference in the resistances of the channel in the on state and the off state, a large difference is essential for good switching operation. And from **Figure 10** it is evident that to maintain a ratio of at least 3-4 orders of magnitude for the two devices, one must set an In composition of $\sim 20\%$ or less.

The final metric that determines the ability of the device to produce a current change with minimum applied voltage is the subthreshold swing (SS). It is the measure of the channel and its electrostatic control, as well as the quality of the interface and associated interface trap density. A SS of 100 mV/dec implies a change of 1 order of magnitude in the drain current upon application of 100 mV at the gate. Considering the interface trap density used in the calibration models for Ge and InGaAs (see previous discussion on the model calibration), the SS cannot reach its best possible value of 60mV/dec at room temperature. The SS for the two devices is summarized in **Figure 11**, and a relative independence for the SS values is seen for In composition up to 40 %. This indicates that a SS of 90-100 mV/dec can be expected for the two devices. With further

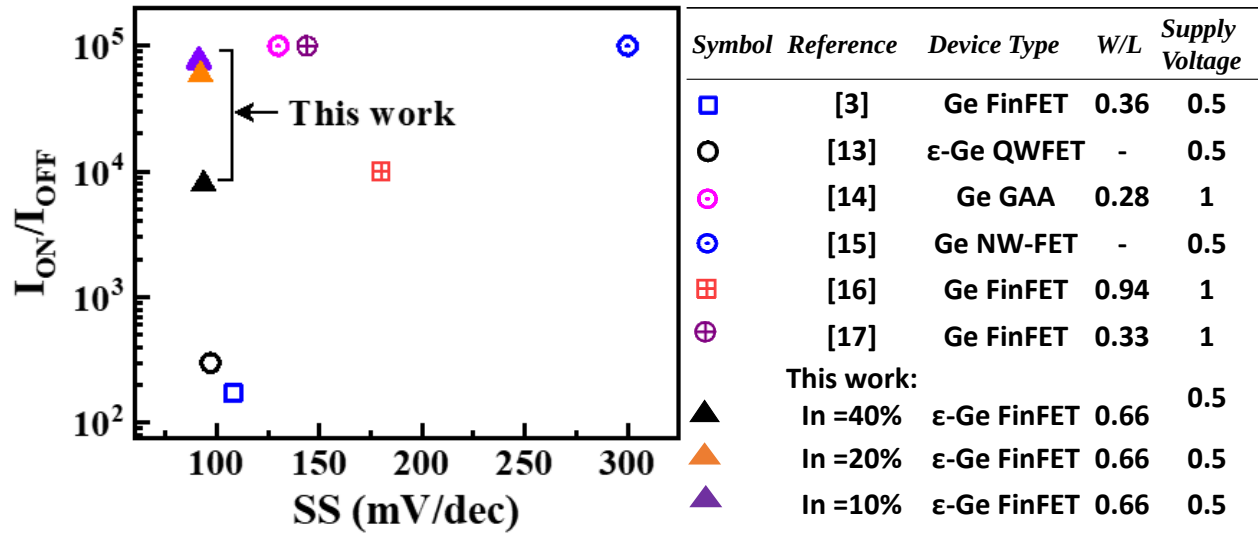


Figure 12. Benchmarking of the tensile strained Ge p-FinFET performance metrics with other Ge reports.

exploration and interface engineering for the Ge-OX interface and the InGaAs-OX interface, a reduction in D_{it} is possible bringing it closer to the ideal values obtained in Si FETs. This will consequently bring down the SS also to the ideal Si state-of-the-art levels of $\sim 60\text{mV/dec}$.

Lastly, the tensile strained Ge p-FinFET and its strain dependence is the first of its kind report, so a benchmarking with other state-of-the-art research works [3, 13-17] is provided in **Figure 12**. It is evident that the Ge p-FinFET provides an excellent SS and on-off current ratio for a scaled voltage of 0.5V.

3.4 CMOS circuit simulation: Methodology and Metrics

For single-material long channel CMOS circuits, in order to have a noise-immune and symmetric response, equal V_T and I_{ON} are sufficient criteria for the n-FET and p-FET. However, for the proposed co-integrated CMOS system, the In composition affects the device performance of the n-FinFET and p-FinFET in distinct and interdependent ways, as discussed in the previous section. Thus, the dc and transient response is evaluated with these device structures using the mixed-mode solver in the Sentaurus device simulator. This enables the complete solution of both the devices along with the interconnects and parasitics. The dominant parasitics, gate and diffusion

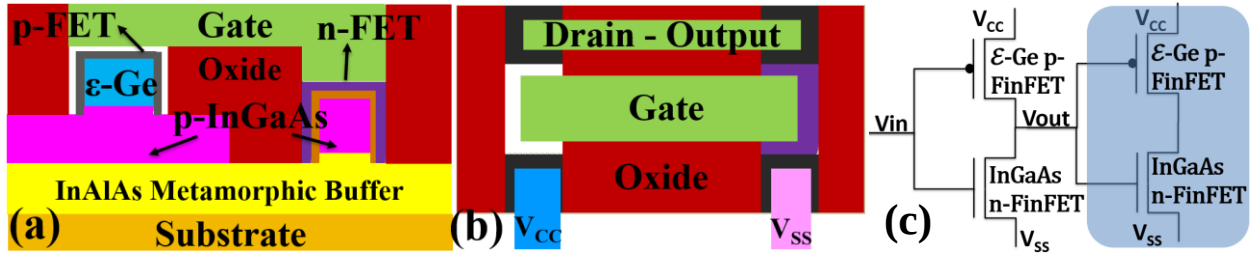


Figure 13. (a) The cross-section view for the proposed cointegrated CMOS inverter formed by a tensile Ge p-FinFET and InGaAs n-FinFET, as well as the interconnect. (b) the top view of this inverter, and (c) schematic representation of the CMOS inverter DUT driving a fan-out load of 1.

capacitances (DUT as well as fan out load), are incorporated through the calibrated model as real-time physics-dependent quantities. The cross-sectional layout of co-integrated CMOS inverter is shown in **Figure 13**. The schematic representation of the fan-out 1 load configuration for the CMOS inverter DUT is also shown in **Figure 13**. An ideal lossless interconnect has been realized through a SPICE-style connection within the simulation framework for the routing.

An important metric for CMOS logic circuits is noise margin (NM) and it can be evaluated through a quasi-stationary DC ramp for the CMOS inverter. Ideally, we expect $V_{IL} = V_{IH} = V_M = V_{CC}/2$ to have noise-immune function ($NM_H \sim NM_L \sim V_{CC}/2$) [18]. Hence, it is advantageous to have V_{IH} as close as possible to V_{IL} and this value to be halfway between the operational rails, V_{OL} to V_{OH} . This implies that the inverter switches abruptly; and that the gain in the transition region is high. For a V_{CC} of 0.5 V (as well as V_{in}), the crossover point V_M needs to be ~ 0.25 V. The physical models of the n-FinFET and p-FinFET are solved simultaneously to study the DC performance of a CMOS inverter for each In composition. Noise margins NM_H and NM_L as well as V_M diverge from their optimal value of $V_{CC}/2$ above and below In composition of $\sim 20\%$ as

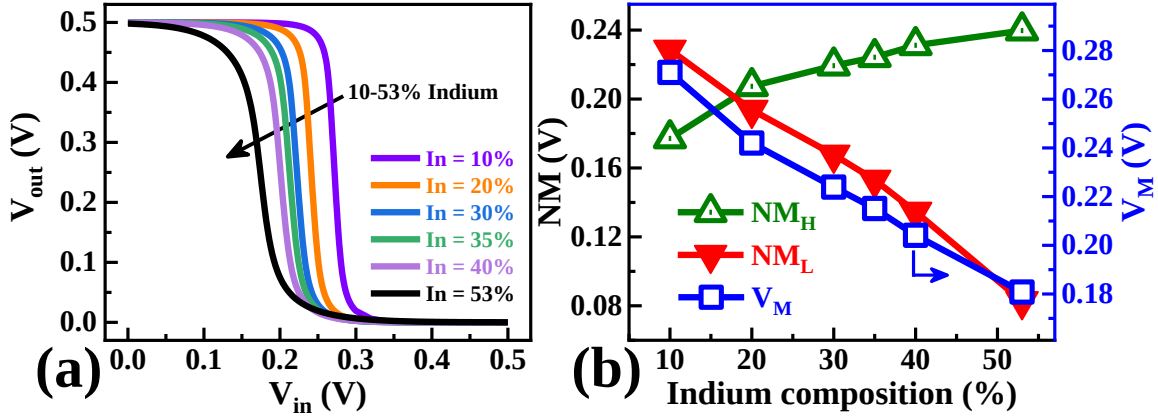


Figure 14. (a) DC transfer curve for the cointegrated CMOS inverter and the corresponding shift in the switched threshold, (b) corresponding extracted noise margins and the inverter switching voltage V_M .

shown in **Figure 14**. The ideal V_M of $V_{CC}/2$ for the CMOS inverter is expected to be around 35 % In based on the V_T match seen earlier, but that does not hold true with V_T roll-off and short channel effects seen in FinFETs [19]. The most noise-immune configuration lies in the vicinity of 15 - 20 % In. Increasing the In composition from 10 - 53% is seen to shift the transfer curve to the left indicating a stronger n-FET operation. This is expected as the InGaAs mobility is very large at high In composition and the bandgap is also sufficiently low.

The cumulative performance and suitability for HPC CMOS applications, the transient response of the CMOS circuits such as inverter, inverter DUT driving a fan out load, CMOS standard cells such as NAND, ring oscillators and SRAM cells is required. This can give a true idea about the drive, leakage, power consumption, delay, power delay product and operating

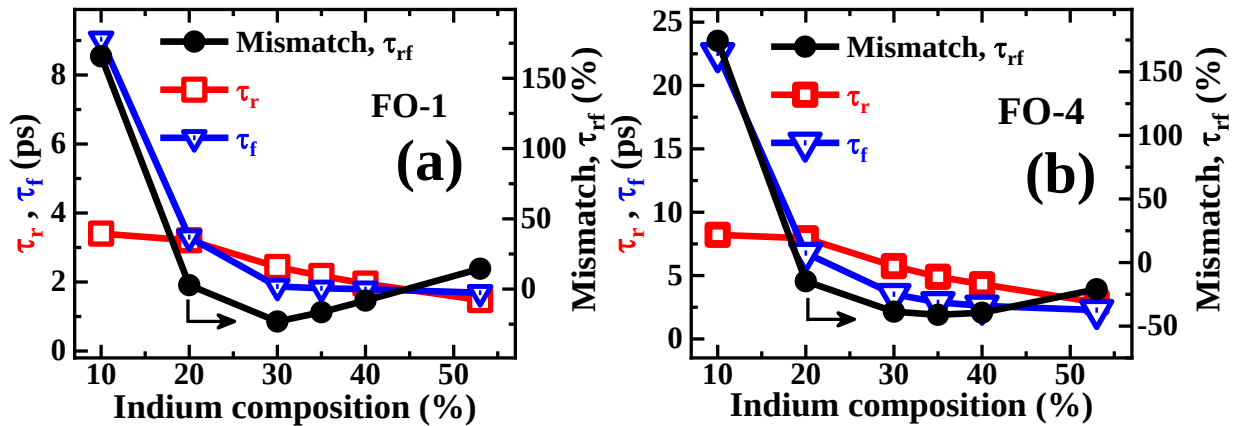


Figure 15. Transient response CMOS inverter: Rise and fall time as a function of In composition for (a) FO1 and (b) FO4.

frequency. By inputting a sharp pulse to the DUT, while driving a sufficient load, one can test the transient response. A configuration where the DUT drives an instantiation of itself is called fan-out 1 or FO1. Similarly, a configuration where the DUT drives multiple instantiations of itself is called FO3 or FO4. The τ_r and τ_f are calculated considering a 0 - 90 % rise and 90 - 0 % fall in the output voltage upon application of a sharp square pulse as input to the CMOS inverter. The rise and fall times, as well as the mismatch between the rise and fall times are presented as a function of In composition for the cointegrated CMOS inverter in the FO1 and FO4 configuration are shown in **Figure 15**. One can note that the rise and fall times increase drastically while moving from FO1 to FO4, this is a consequence of the large load and the associated large RC delays with it. Between 20 - 40% In composition, it is evident that the rise and fall times are minimal and nearly matched. The mismatch can be positive or negative depending on which path is stronger, the Ge p-FinFET pull-up path or the InGaAs n-FinFET pull-down path. A rise and fall time of roughly 2-3 ps is

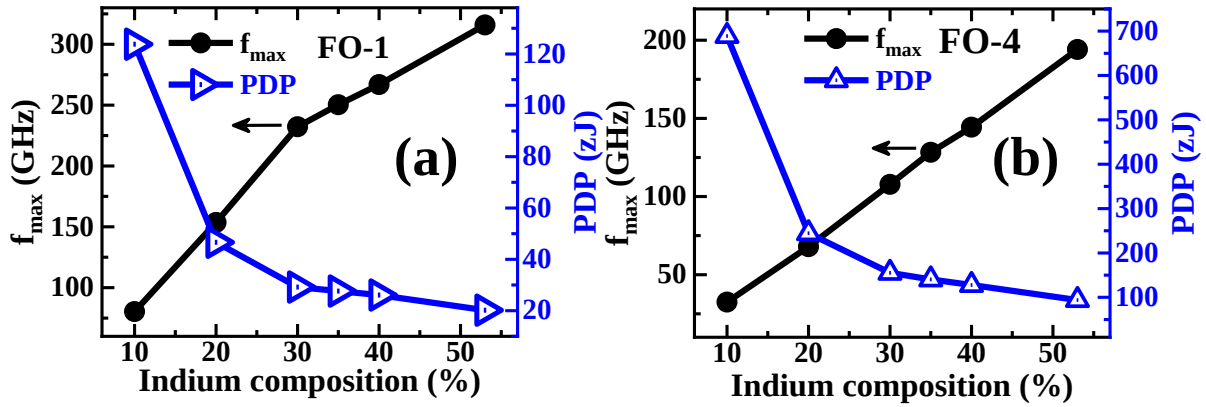


Figure 16. Maximum switching frequency and the corresponding consumed total PDP as a function of different In composition for the cointegrated CMOS inverter. (a) FO1 and (b) FO4.

present in the FO1 configuration, whereas it rises to ~ 5 ps for the FO4 configuration. The fall time associated with the pull-down path of the InGaAs n-FinFET is very large at low In composition due to the large bandgap of InGaAs and the associated low drive current. Note that the drive current for the InGaAs n-FinFET was much lower than the Ge p-FinFET as seen in **Figure 8**. Thus, the overall decreasing trend for the rise and fall times with increasing In composition can be attributed to the improved/boosted on currents associated with the lowering of bandgaps and increase of mobilities of both the channels.

While driving a FO1 or FO4 load, the cointegrated CMOS inverter DUT is tested for a maximum possible switching frequency as part of a high-resolution transient simulation. As the switching frequency is increased, a large rise in the power consumption. This power is contributed largely by dynamic power consumption and the short circuit current, there is however the leakage static power also included here. The short circuit current induced power dissipation is a problem in all CMOS circuits and is a consequence of the in-complete turn-off of the complementary devices resulting in a short period where both the devices are partially on. A large delay introduced by the DUT indicates a poor drive and a correspondingly low switching frequency (inversely related to the delay). Although a large switching frequency is expected while driving the desired load, one must also keep track of the power. To achieve a balance between the frequency/delay

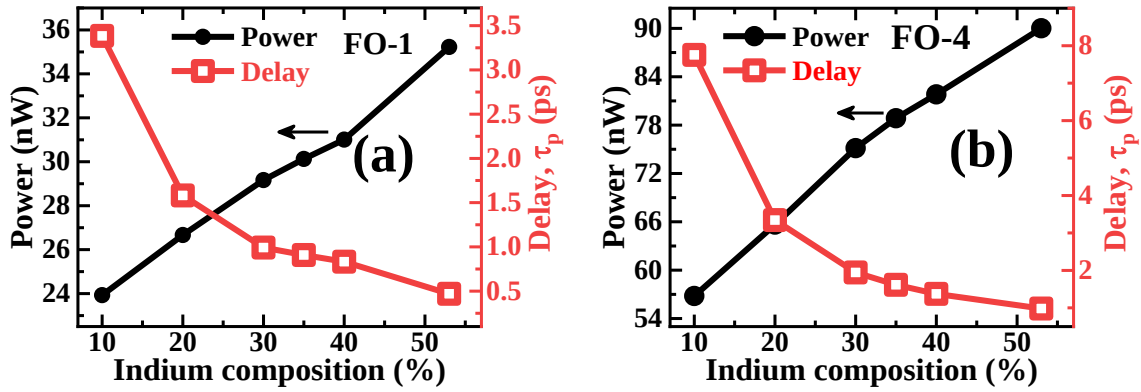


Figure 17. Maximum switching delay and the corresponding consumed total power consumed in 1 cycle as a function of different In composition for the cointegrated CMOS inverter. (a) FO1 and (b) FO4.

and the total power consumed, a quantity called the power delay product (PDP) is defined. The PDP and the switching frequency for the cointegrated CMOS inverter in the FO1 and FO4 configurations are summarized in **Figure 16**. As the In composition increases, the drive strength for both devices improves as seen earlier, resulting in faster operation and hence an almost linear increase in the frequency of operation/switching. The PDP improves rapidly initially due to the faster operational and reduced delays, but the power eventually rises faster resulting in a negligible improvement in PDP beyond $\sim 20\%$. **Figure 17** visualizes the individual delays and power consumed in one cycle by the cointegrated CMOS inverter. Power consumption down to 26 nW for the FO1 and 66 nW for the FO4 is attainable in the vicinity of $\text{In} = 20\%$. Similarly, gate delays down to 1.5 ps for the FO1 and 3 ps are attainable in the vicinity of $\text{In} = 20\%$. Total power

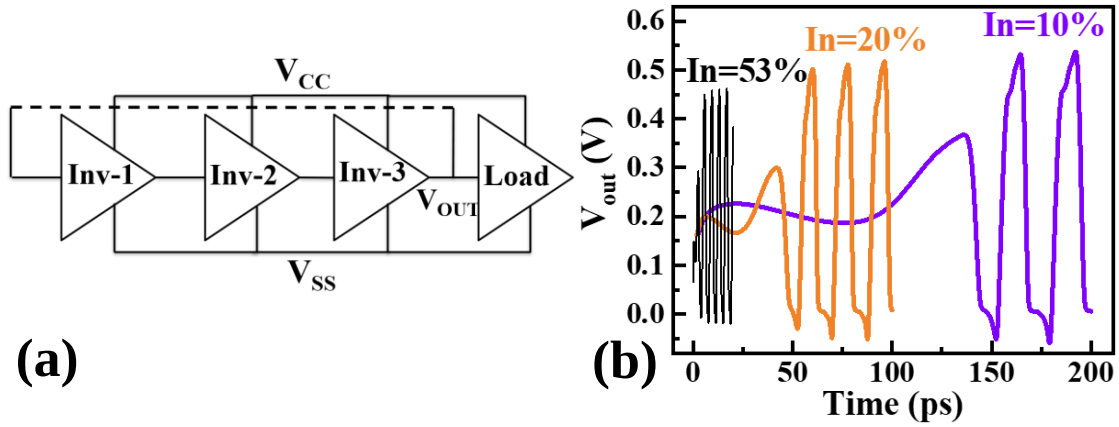


Figure 18. (a) Schematic for a 3-stage ring oscillator made using the cointegrated CMOS inverters, (b) transient response for the ring oscillator for three different In composition to visualize the settling time and oscillation frequency.

dissipation through static leakage, switching and short circuit path is calculated using the instantaneous transient current drawn from the power supply and discussed in **Figure 16** and **Figure 17**. Below 20 %, the transition time mismatch has a sharp increase for lower In, beyond 40 % the trend points towards increasing mismatch between pull-up and pull-down paths and eventual hard failure beyond 53 % (data not shown here), due to high strain and low bandgap. To obtain a symmetric response, there are two values of In where the rise and fall times match exactly; one value lies in the vicinity of 20 % and the other value lies near 40 %.

The performance of a 3-stage CMOS ring oscillator (schematic is shown in **Figure 18**) is tested using the proposed co-integrated inverter DUT while assuming ideal lossless interconnects

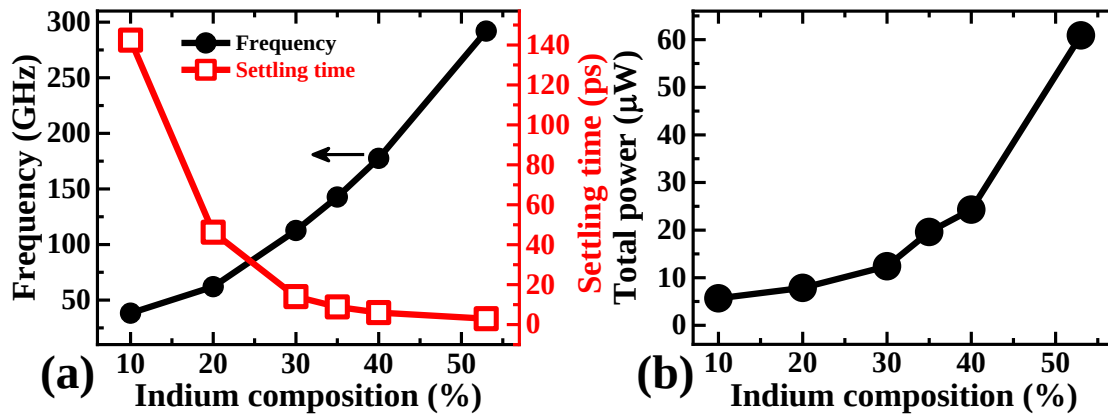


Figure 19. (a) Oscillation frequency and settling time for the ring oscillator, (b) total power consumed by the 3-stage ring oscillator.

between the proposed devices. The transient response is shown in **Figure 18**, indicating a significant increase in operating frequency and power while showing a reduction in settling time with an increase in the In composition as shown in **Figure 19**, respectively. The rail-to-rail swing reduces with higher In compositions beyond 40 %, as seen in **Figure 18**. The possible operating frequency of the output lies in the range of 50 - 300 GHz in the FO-1 configuration. The settling time for stable and peak-to-peak oscillations is an important merit for oscillators and clock generation circuits in the context of power management in LSI chips indicating a faster power-on time for the ring oscillator at higher In at the cost of higher power dissipation.

3.5 Interdependent performance of the cointegrated CMOS: A summary

Based on the results discussed in this section it is evident that the cointegrated CMOS system provides many desirable metrics. Here, a summary is provided pictorially representing how the In composition affects the device and circuit performance as well as the various metrics. The summary is shown in **Figure 20**. The bandgap of $\text{In}_x\text{Ga}_{1-x}\text{As}$ at low In is high (~ 1.3 eV at In =

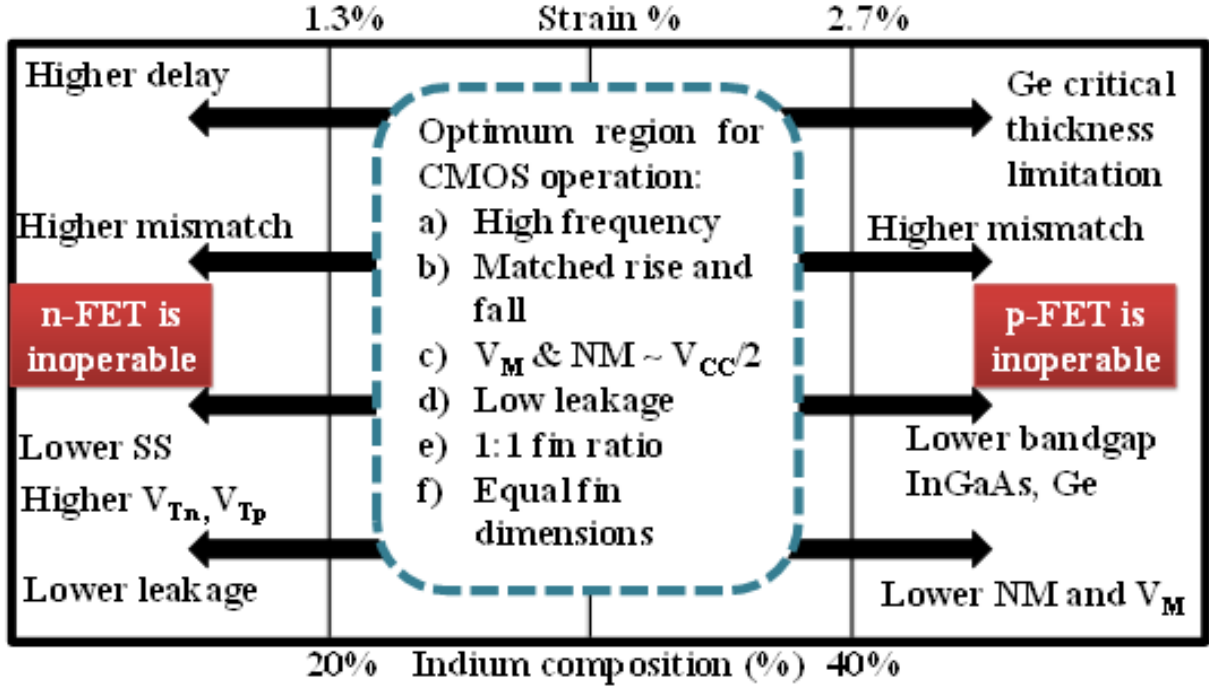


Figure 20. Summary of the design consideration for the tensile Ge p-FinFET and InGaAs cointegrated CMOS system from a device and circuit perspective. The complete CMOS operation is seen to be optimal and tunable in the range of In composition from 20-40 %. The impact of the In composition on all the device and circuit metrics is summarized.

10%) indicating a high V_T (~ 0.5 V), lower I_{OFF} and improved I_{ON}/I_{OFF} ratio. At this high V_T , the CMOS device is inoperable at V_{cc} of 0.5 V, providing a lower bound for In composition. In both devices, an arbitrarily high In composition is undesirable as it degrades the leakage current significantly. Thus, there should be a range of In composition for ϵ -Ge/InGaAs CMOS architecture where the device performance is optimum. The n-FinFET device reported in Ref. [11] utilizes In composition of 53 %, which corresponds to a tensile strain on the Ge epi-layer of ~ 3.3 % and the bandgap becomes ~ 0.1 eV. Thus, at such a high value of tensile strain, Ge fails to be a candidate for p-FinFET channel material since it has extremely high leakage as shown in **Figure 9**. In

addition, the critical thickness of Ge reduces with higher In composition, as discussed earlier, limiting the fin height of the Ge p-FinFET. These two factors provide an upper bound for the choice of In composition in this co-integrated CMOS structure.

The ideal V_M of $V_{CC}/2$ for the CMOS inverter is expected to be around 35 % In based on the V_T match seen earlier, but that does not hold true with V_T roll-off and short channel effects seen in FinFETs [19]. While the most noise-immune configuration lies in the vicinity of 20 % In. In the range of values of In between 20 - 40 %, the rise (τ_r) and fall (τ_f) times for an inverter tend to be close implying that the transition asymmetry tends to be near-zero in this range.

The leakage increases and NM degrades drastically as In increases. Thus, it is advantageous to maintain a composition of ~ 20 % for optimum and matched response with low leakage and good NM. The τ_p drops significantly between 20 - 40 providing an operating frequency boost at the cost of power and NM. Therefore, at ~ 20 % In, the power, τ_p (f_{max}) and NM are optimum, for equal fin dimensions of the n-FinFET and p-FinFET ($L = 60$ nm, $W = 40$ nm, $H = 40$ nm), while maintaining a 1:1 fin ratio in FO-1 and FO-4 load configurations. Moreover, the fin height of the Ge p-FinFET at this In composition is realizable considering the critical layer thickness for this ϵ -Ge on $In_xGa_{1-x}As$ system [4]. The device parameters such as, V_T , I_{ON} , I_{OFF} , and SS for Ge p-FinFET and InGaAs n-FinFET were analyzed with identical fin dimensions as a function of In composition, and summarized in **Figure 20**. These parameters have a strong dependence on the In composition, where I_{ON} of both devices increases, I_{ON}/I_{OFF} and SS degrade with increasing In composition. This is due to the decrease in the bandgap of $In_xGa_{1-x}As$ and the increase in tensile strain on Ge. The tensile strained Ge p-FinFET was benchmarked with other competing architectures and shows superior performance. The matched, noise-immune, and power-efficient CMOS inverter performance was demonstrated over a range of 20 % to 40 % In. Furthermore, a 3-stage ring oscillator was realized with the proposed co-integrated CMOS structure.

3.6 Scaling to advanced N5 node: InGaAs n-FinFET & Tensile Ge p-FinFET

Now that the impact of the most important material parameter in this cointegrated system, i.e., In composition is understood, the discussion can proceed to considerations of device geometry and scaling toward more advanced short channel nodes such as N5 [12]. This section proceeds to evaluate the performance of this cointegrated CMOS system to reveal a cumulative design perspective for geometry scaling and doping variation in the context of a tunable In composition. Often, it is difficult to have intrinsic channels for these III-V materials and Ge, unlike Si, so a detailed understanding of scaling, doping and In composition is presented here. As the length is scaled down from 100 nm to 30 nm, the electrostatic considerations and the control over the channel reduces. The choice of In composition and N_{CH} directly affects the material properties, and thus the application-specific selection of these parameters can lead to a significant impact on the designed CMOS circuit/system. In addition, channel length scaling introduces SCE (*i.e.*, V_{TH} roll-off, increase in SS and DIBL), which further affects the optimum region of operation in terms of In composition and N_{CH} . The cumulative effect of N_{CH} and In composition on the device performance and operability is magnified at shorter channels. DIBL and SS need to be quantified and their dependence on the length, channel doping and In composition is seen for the InGaAs n-FinFET. The results are displayed through contours in **Figure 21** as a means to effectively visualize the relative trends of the metrics for a large number of parameter combinations, while also providing an estimate of the variability due to changes in process, material, and design.

The In composition affects the $In_xGa_{1-x}As$ channel resulting in a spectrum of tunable material properties to utilize for the n-FinFET. A higher In composition results in a lower bandgap

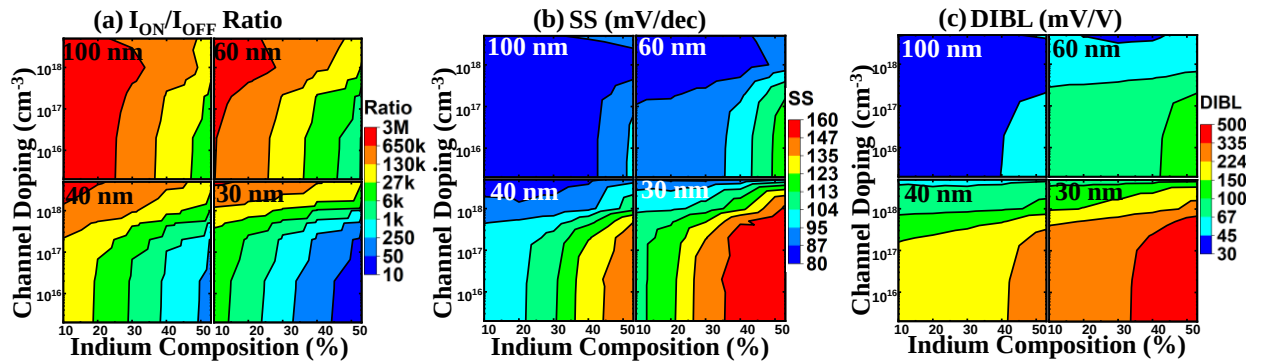


Figure 21. Impact of length scaling for the InGaAs n-FinFET, (a) on-off ratio, (b) SS and (c) DIBL.

in $\text{In}_x\text{Ga}_{1-x}\text{As}$ as well as higher electron mobility. The lower bandgap results in a reduced V_{TH} while the higher electron mobility enhances the I_{ON} ; whereas, a higher N_{CH} increases the V_{TH} . Thus, the In composition and N_{CH} act as competing mechanisms affecting the device performance in opposite ways. For the operation of the n-FinFET at the desired supply voltage of 0.5 V, the V_{TH} must be well within this range (0-0.5 V). The $\text{In}_x\text{Ga}_{1-x}\text{As}$ n-FinFET shows an excellent $I_{\text{ON}}/I_{\text{OFF}}$ ratio for a wide range of In compositions and N_{CH} , indicating suitability for ultra-low power applications. At a high In of 53 %, the bandgap of $\text{In}_x\text{Ga}_{1-x}\text{As}$ decreases significantly, resulting in much higher I_{OFF} . Due to the increase in electron mobility with increasing In composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$, the I_{ON} increases, but the increase in I_{OFF} is much more severe, resulting in an overall degradation in $I_{\text{ON}}/I_{\text{OFF}}$ ratio. There exists a trade-off between the leakage and the drive strength for the $\text{In}_x\text{Ga}_{1-x}\text{As}$ n-FinFET. For In = 10 % with $L = 40$ nm, I_{OFF} is ~ 8 pA/ μm and becomes ~ 20 nA/ μm at In = 40 %, indicating a $2500\times$ increase in I_{OFF} . On the other hand, the I_{ON} is ~ 2 $\mu\text{A}/\mu\text{m}$ at In = 10 % and becomes 135 $\mu\text{A}/\mu\text{m}$ at In = 40 %, indicating a $67.5\times$ increase in I_{ON} . Although the device can now drive larger loads faster due to high I_{ON} , the I_{OFF} has increased drastically resulting in a decrease in $I_{\text{ON}}/I_{\text{OFF}}$ ratio.

Approaching shorter gate lengths is expected to exacerbate SCE as the L is varied from 100 nm to 30 nm. **Figure 21** shows the SS and DIBL as a function of In and N_{CH} , respectively. The devices with longer channels remain immune to SCE and this can be seen by the *blue-shades* indicating low values of SS and DIBL. Furthermore, it can be seen that the performance of short-channel devices is more sensitive to variations in the In composition and doping compared to long-channel devices. With increasing In composition, the I_{OFF} rises significantly, resulting in higher

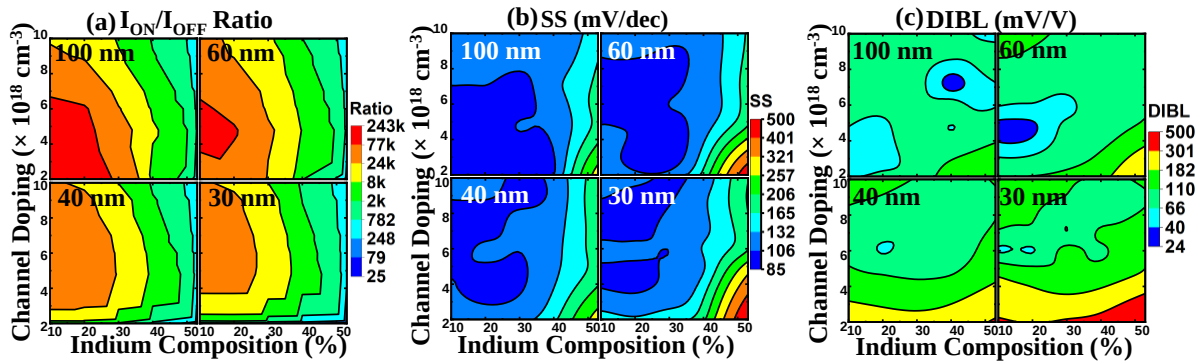


Figure 22. Impact of length scaling for the tensile Ge p-FinFET, (a) on-off ratio, (b) SS and (c) DIBL.

leakage and hence a degraded SS. The shift in the contours toward the *top-left corner*, indicates that a higher N_{CH} is required to mitigate the SCE, thus improving DIBL and I_{ON}/I_{OFF} ratio at a channel length of 30 nm. Additionally, in device configurations having high I_n and low N_{CH} (see, *bottom-right corners*), the SCE dominate the device performance, as seen through the degradation of SS and DIBL. Further length scaling is possible through reduction of W and corresponding improvement in electrostatic control. Based on the results shown here, the optimum N_{CH} of $5 \times 10^{17} \text{ cm}^{-3}$ is used for further analysis. At this N_{CH} , the $\text{In}_x\text{Ga}_{1-x}\text{As}$ n-FinFET shows excellent CMOS operation and performance at 0.5 V.

The In composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$ indirectly creates a spectrum of material properties through the tensile strain in Ge (bandgap and hole mobility). The hole mobility increases and the bandgap decreases with increase in tensile strain in Ge [20], resulting in an increase in I_{ON} and I_{OFF} . Also, the absolute leakage in $\varepsilon\text{-Ge}$ is expected to be higher than $\text{In}_x\text{Ga}_{1-x}\text{As}$ as the bandgap is lower in Ge, resulting in a lower I_{ON}/I_{OFF} ratio. **Figure 22** shows the interplay between the competing variables, In composition and N_{CH} , and their effect on device performance. A relatively low N_{CH} has the advantage of reduced impurity scattering but results in low V_{TH} , and reduced I_{ON}/I_{OFF} ratio. With increasing In composition, the bandgap of Ge reduces, resulting in lower I_{ON}/I_{OFF} ratio. Thus, warranting a careful optimization of the Ge p-FinFET channel doping and In composition in order to obtain the desired operability and performance. Devices with channel

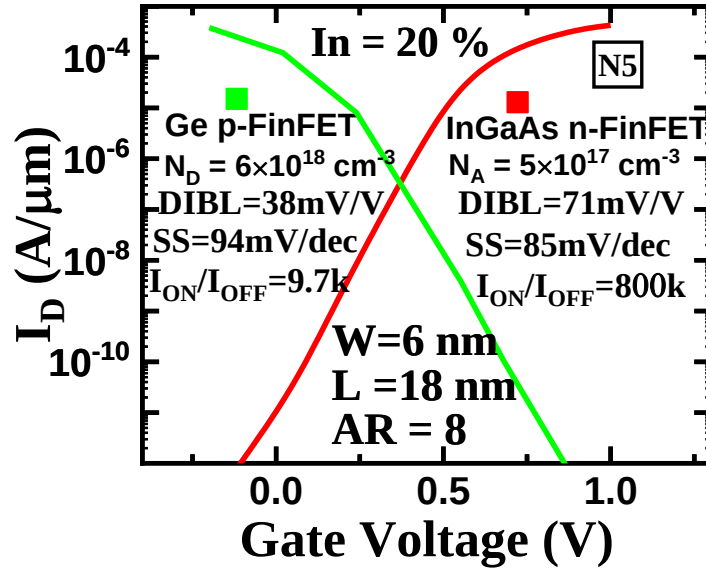


Figure 23. Performance and metrics for the optimized tensile Ge p-FinFET and InGaAs n-FinFET at the N5 node along with the performance metrics at $\text{In} = 20 \%$.

lengths of 30 nm and 40 nm require a higher N_{CH} to mitigate the degradation of DIBL, SS, and I_{ON}/I_{OFF} ratio due to length scaling. The SS, DIBL, and I_{ON}/I_{OFF} ratio at lower N_{CH} degrade more rapidly with increasing In composition due to increased SCE, as seen through the SS and DIBL variation. The SS indicates the switching slope due to the low bandgap nature of Ge, along with a realistic interface trap density, to maintain normally-off operation with a good I_{ON}/I_{OFF} ratio for p-FinFET, high N_{CH} as well as a large work function metal are needed. The TiN gate metal work-function of 4.5 eV was selected here to provide a higher I_{ON}/I_{OFF} ratio and V_{TH} and reduce the requirement of high N_{CH} (exotic gate metals can relax this dependency further). For optimum p-FinFET design, the device performance *i.e.*, $V_{TH} < 0$, I_{ON}/I_{OFF} ratio > 1000 as well as low SS and DIBL should be achieved while keeping N_{CH} as low as possible (*here*, N_{CH} of $6 \times 10^{18} \text{ cm}^{-3}$ is chosen).

Finally, after understanding the scaling trends for the two complementary devices, the optimized performance for the N5 node can be seen in **Figure 23**.

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Chapter 4 – Ge-on-AlAs lattice matched Nanosheet-FET

4.1 Sub-3 nm IRDS roadmap: NSFETs beyond FinFETs and outlook

After exploring the tri-gate FinFET based Ge and InGaAs monolithic CMOS devices in the previous section, an exploration of the Ge epitaxial system to more advanced nodes is presented in this section. This Ge epitaxial system can also fit well beyond the N5 node in the IRDS roadmap as the transistor architecture moves from tri-gate FinFET devices to quad-gate gate-all-around Nanosheet-FET (NSFETs). A FinFET has electrostatic control over the channel from 3 directions, whereas the NSFET has control from all 4 sides of the channel. Beyond the 3 nm FinFET node, further reduction in device footprint as well as improvement in device performance is possible by transitioning from FinFET to a gate-all-around (GAA) architecture [1]. In addition to the improved electrostatics provided by the GAA architecture, a vertical 3D stacking of devices is required to improve the chip integration density as well as individual device performance. As the industry unveils one of the first Si GAA based designs [2]-[4], one must look for alternative design and process solutions to ensure sustained scaling of this technology to future high-performance and low-power computing. Approaching atomic dimensions aggravates pre-existing issues such as quantum confinement induced changes in the bandgap, effective mass, and mobility as well as short channel effects (SCE): drain induced barrier lowering (DIBL) and subthreshold swing (SS). The GAA nanosheet FET (NSFET) can be fabricated using the existing process and design infrastructure of the FinFET while providing a performance boost and higher effective width [2]-[4]. In addition, the variability of the NS thickness is minimal as it is determined during epitaxy, whereas the fin height is determined by etching, thus making the NSFET performance more reliable and immune to random variations [2].

There are five ways to improve the drive capabilities of NSFET-based CMOS devices: alternate/modified channel material, parallel connection of multiple devices, wider device, thicker sheet, and higher number of vertically stacked NS (N). Each of these, except the last, are design constraints shared with the FinFET and all of them have distinct effects on the performance of scaled NSFETs in terms of parasitics, threshold voltage (V_{TH}), SS, DIBL, I_{ON} , and I_{ON}/I_{OFF} ratio, while posing unique process and design challenges. One of the reasons for the success of Si-based p-FinFET over the years has been the high hole mobility for the (110) orientated crystallographic plane, resulting in improved performance of taller fins [4]. As we approach shorter and wider

Node	Nanosheet Dimensions (L,H,W) in nm
N2.1 HP	(14,7,30)
N2.1 HD	(14,7,15)
N2.1 SRAM	(14,7,7)
N1.5 HP	(12,6,25)
N1.5 HD	(12,6,11)
N1.5 SRAM	(12,6,6)
N1 HP	(12,5,20)
N1 HD	(12,5,6)
N1 SRAM	(12,5,6)
N0.7 HP	(12,5,15)
N0.7 HD	(12,5,6)
N0.7 SRAM	(12,5,6)

Figure 24. The various projected advanced nodes according to IRDS, all of which are GAA NSFET structures.

channel devices, like the Si NSFET or nanowire-FET (NWFET), this advantage will be lost due to the lower surface area of (110) plane, this warrants the use of higher hole mobility channel material. Germanium offers 4× higher hole mobility than Si and exploration of Ge-based NSFET

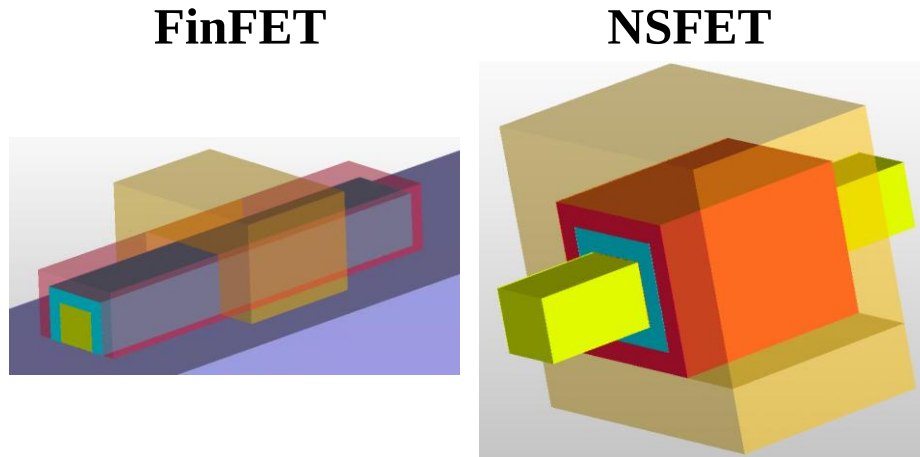


Figure 25. The expected structure for a FinFET (left) and a NSFET(right). The source and drain regions have been omitted in this illustration for simplicity. The orange region surrounding the channel is the gate metal, TiN. The red-region underneath the metal is the high-k dielectric HfO₂ and the light-blue region further inside is the interfacial oxide such as SiO₂ or GeO_x. The innermost yellow-region is the channel made of Ge. The FinFET structure has a template layer below it shown by the purple-region, here it is GaAs or InGaAs.

with higher hole mobility will provide superior device performance. A complete physics-based calibrated-model informed analysis of this new Ge NSFET system, process, drive and trade-offs is possible when the design is taken to a circuit or unit cell level. This enables testing and characterization of standard cell transient, DC, and noise metrics, which are ultimately what matter for large-scale system integration. The projected dimensions (L, W, H) of the various advanced nodes up to the Angstrom regime, are shown below in **Figure 24** according to IRDS. The typical structure for a FinFET and NSFET is shown in **Figure 25**.

4.2 Ge NSFET fab process: Lattice matching and AlAs sacrificial layers

The advantages of using a Ge high mobility channel have been known for more than a decade [5], but so have the process challenges faced while fabricating and operating Ge-based devices compared to Si devices. Process hurdles, defects, and interface issues for Ge devices have outweighed the benefits provided compared to Si. But at the end of this roadmap, Si devices have moved to an NSFET-CFET regime where further performance scaling is slow, the cost of improvement is very large and the fabrication process is defect-prone leading to major yield issues [1, 2]. As the industry progresses toward large-scale deployment of advanced NSFET in the coming years and CFET around 2034 with Si channel devices [1], this work looks for an alternative solution using Ge where significant process and performance advantage can be obtained over their Si counterparts. One of the major advantages of Si devices, which has led to major process and yield success over the past decades, is the single-crystal ultra-defect-free Si substrates. Defect and unwanted strain-free channels lead to reliable transistor operation as well as good interface properties. This advantage is often difficult to incorporate in other semiconductors such as carbon-nanotubes, MoS₂, III-V compounds, Ge or GeSn. The next best thing that is often used in making non-Si optoelectronic devices is homoepitaxy and lattice matching achieved through careful epitaxial growth. However, the fabrication of Si NSFETs relies on a Si/SiGe multilayer heteroepitaxial growth following a SiGe-graded buffer, which results in a tensile strain ($\sim 1 - 1.5\%$) in the stack due to significant lattice mismatch between Si and the Si_{0.7}Ge_{0.3} layer [3, 5]. This structure drifts away from the benefits of having single crystal Si as the channel. Although this strain may benefit device performance, it introduces a crucial constraint on the height of the device as well as the number of vertically stacked layers. For a better drive current, the devices would tend to be designed to have a larger height, but beyond a specific height, called the critical layer thickness, the pseudomorphic stack starts to relax the strain, resulting in an exponential rise in defects and dislocations [5]. The process for the Si NSFET fabrication, as will be discussed in this section, relies on the etching of the underlying alternating SiGe sacrificial layer. The Si channels grown on these SiGe sacrificial layers are strained due to the lattice mismatch, and once these layers are removed, the lattice condition of the Si channels is relaxed by an unknown amount. This unknown relaxation is most likely plastic and results in a large number of defects and dislocation in the channels. The alternative to this is to grow the Si/SiGe multilayer heteroepitaxial while

ensuring intentional and complete relaxation of all the layers involved during the epi-growth, before the etch. Although, through process optimization, this can ensure that there is no concern of strain relaxation after the etch, a relaxation before the etch is equally harmful in terms of defects. Regardless, both methods of fabricating the Si/SiGe multilayer heteroepitaxial NSFET require an intentional strain relaxation process step. The growth of thick layers of epitaxial films is possible by growing a defect-absorbing layer followed by a defect-free layer by leveraging optimized growth recipes and annealing steps. However, this is especially challenging for tiny epi-layers of 5-10 nm like the layers needed for the Si/SiGe multilayer heteroepitaxial NSFET fabrication. In addition, the sacrificial layer, *usually* $\text{Si}_{0.7}\text{Ge}_{0.3}$, should provide a high etch selectivity with respect to the active Si channel to ensure minimal loss of Si during fabrication [3] and complete removal of the unwanted sacrificial layers of $\text{Si}_{0.7}\text{Ge}_{0.3}$. Any left-over residue of the sacrificial layer can participate in parasitic conduction, and leakage as well as reduce channel electrostatics.

The starting epitaxial layer stack used for the fabrication of Si NSFETs which utilizes a Si/ $\text{Si}_{0.7}\text{Ge}_{0.3}$ is shown in **Figure 26(a)** [3], the layer structure used for Ge channel NSFETs which uses a Ge/Si multilayer stack is shown in **Figure 26(b)** [6], and **Figure 26(c)** is the starting epitaxial

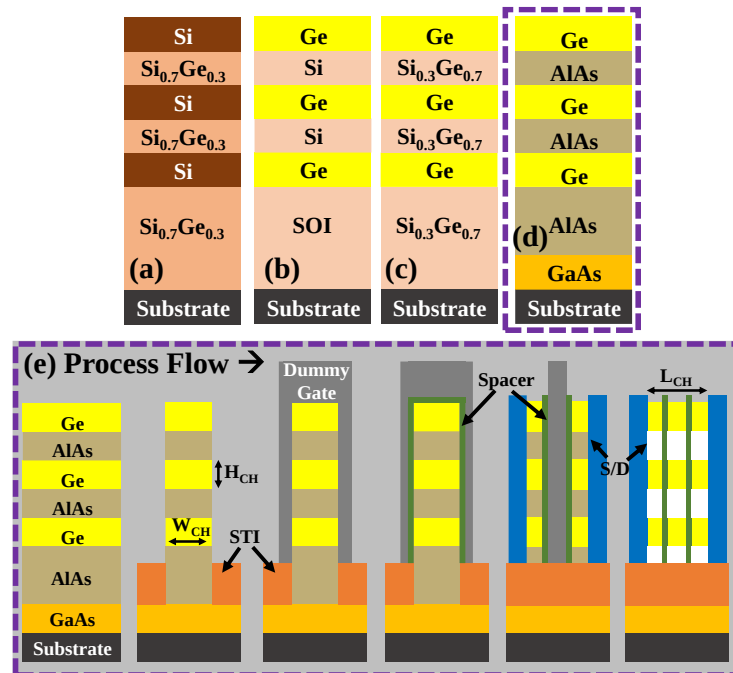


Figure 26. Schematic of (a) conventional epitaxial stack for Si NSFETs, (b) Ge/Si stack for Ge NSFETs, (c) alternative Ge/SiGe starting stack for Ge NSFET, (d) proposed Ge/AlAs epitaxial stack for Ge NSFETs. (e) Proposed process flow for Ge/AlAs lattice matched NSFET fabrication from growth to NS release.

stack used for Ge NSFET which uses a Ge/Si_{0.3}Ge_{0.7} stack [7, 8]. The starting epitaxial stack studied in this work is shown in **Figure 26(d)** which uses a lattice-matched Ge/AlAs multilayer structure. The NSFET fabrication process involves four key steps: (i) multilayer epitaxy with alternate layers of channel material (Si or Ge) and sacrificial layer (SiGe or *here*, AlAs) which defines the thickness, composition and material quality of the of the NSFET channel, (ii) fin patterning and definition of channel length (L_{CH}) and channel width (W_{CH}), (iii) dummy gate and outer spacer deposition for anchoring of the NS followed by source and drain epitaxial growth, and (iv) etching of the sacrificial layer followed by NS release [3, 9]. Utilizing the Si/SiGe multilayer structure (shown in **Figure 26a**) to realize the Si-based NSFETs is possible through pseudomorphic growth [5] and will introduce defects and dislocations due to the possible strain relaxation as discussed earlier. The growth of the first epitaxial Si active region on Si_{0.7}Ge_{0.3} will result in a biaxial tensile strain of 1.1 % in Si. The consequent layers will adhere to the in-plane lattice constant of the Si_{0.7}Ge_{0.3}, provided the total thickness of the subsequent epitaxial layers does not exceed the critical layer thickness associated with strained Si/SiGe growth. In this scenario,

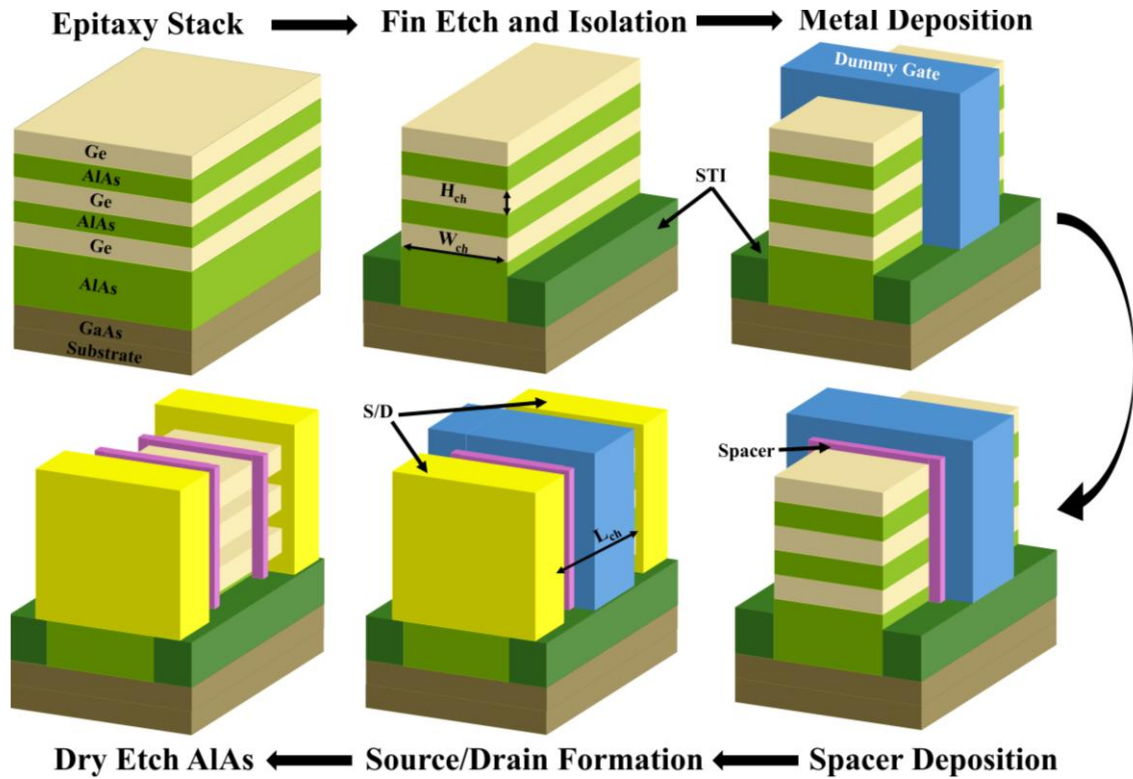


Figure 27. The process flow for lattice matched Ge-on-AlAs NSFET fabrication from epitaxial stack growth to S/D formation and AlAs sacrificial layer removal.

the multilayer epitaxial growth will retain the strain. The critical layer thickness in such a system is ~ 50 nm [5] and beyond this thickness, the system will relax and create defects and dislocations

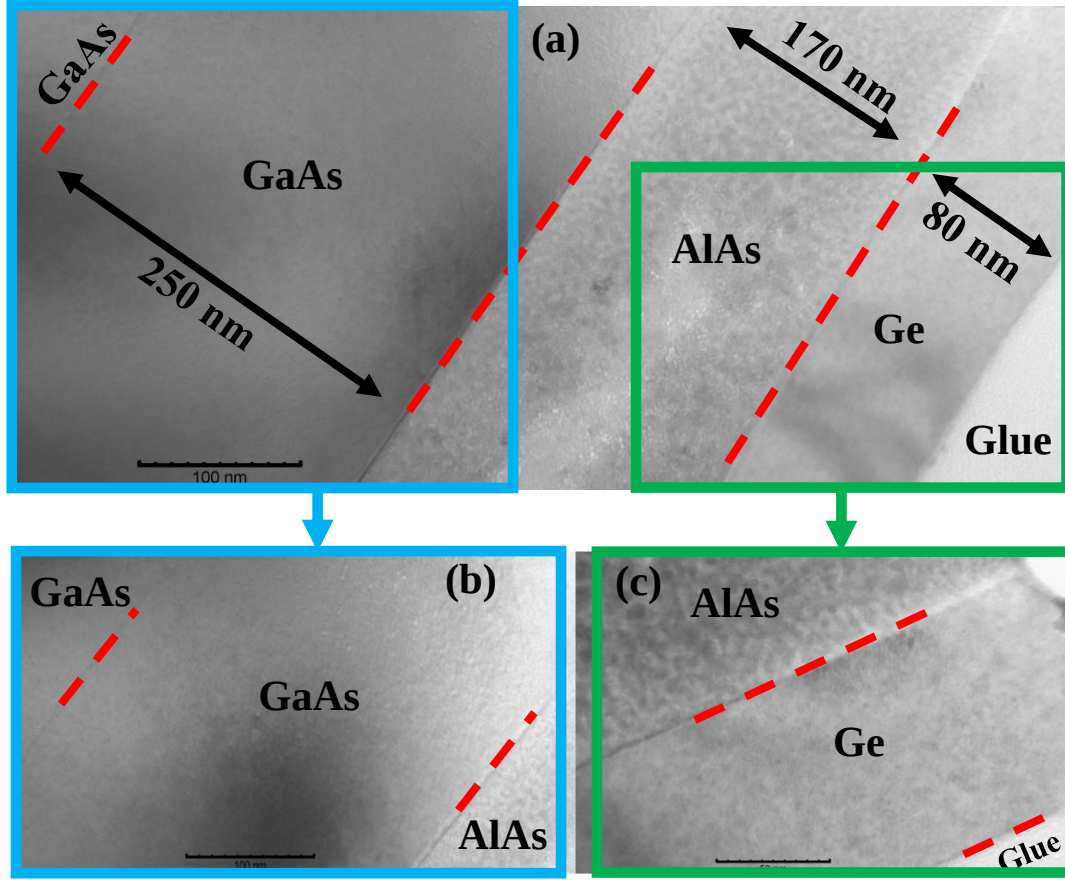


Figure 28. Cross-sectional TEM micrograph of proposed Ge/AlAs lattice matched heterostructure, (a) Ge/AlAs/GaAs with high-quality heterointerfaces, magnified view of (b) AlAs/GaAs, and (c) Ge/AlAs heterointerface.

even before the NS release step. The Ge/Si_{0.3}Ge_{0.7} multilayer structure used for Ge NSFET shown in **Figure 26(c)** [7, 8] will result in similar pseudomorphic Ge growth and thickness constraints. Furthermore, the Ge/Si multilayer structure used for Ge NSFET shown in **Figure 26(b)** [6] will result in a ~ 4 % lattice mismatch, resulting in a further aggravated strain relaxation issue. This limits the total height of the device (*i.e.*, number of stacked layers $\times$ vertical pitch) and restricts the number of stacked layers, vertical pitch as well as the thickness of the individual layer. This constraint is evident through the design guidelines for advanced nodes N2.1, N1.5, N1, and N0.7 [1], which have a vertical pitch of 18 nm, 16 nm, 14 nm, and 14 nm; device height of 53 nm, 48

nm, 57 nm, and 57 nm. To leverage the design and performance benefits of thicker channels and a larger number of stacked channels, the proposed Ge/AlAs can be used, as discussed above. Furthermore, such a system can steer clear of strain relaxation-induced defects in the Ge layer and eliminate the need for dislocation removal anneal steps as well as reliability and yield concerns [10]. A simple schematic for the process flow for Ge NSFET fabrication following a Ge/AlAs multilayer growth is shown in **Figure 26(e)**. The process steps are directly transferrable from Ge FinFET [6] fabrication as well as traditional Si/SiGe NSFETs, except for the selective etch chemistry which can be performed using dry or wet (vapor) etch process. The Ge/AlAs selective etch for Ge NS release can be carried out using a BOE/HF or similar wet-etch chemistry with an extremely high selectivity of $\sim 10^5:1$ resulting in a minimal loss of the Ge active layer, significantly better than the existing $\sim 150:1$ by RIE/dry etch [3], [11], [12] of Si NS. A 3D visualization of the Ge-on-AlAs multilayer NSFET fabrication process, with a few key steps in shown in **Figure 27**.

To demonstrate the excellent material and interface quality of Ge/AlAs/GaAs(100)/2° heterostructure for a Ge-on-AlAs NSFET starting stack, the cross-sectional transmission electron microscopic (TEM) analysis was carried out as shown in **Figure 28**. The epitaxial Ge layer was grown at 400 °C on GaAs with an intermediate AlAs layer by solid- source molecular beam epitaxy. The AlAs buffer layer prevents the atomic interdiffusion of Ge and As, that takes place in a direct Ge/GaAs growth. The high contrast regions delimit the three layers, as shown in **Figure 28(a)** and no defects or dislocations were observed at the AlAs/GaAs (*see Figure 28b*) and Ge/AlAs (*see Figure 28c*) interface, since the entire structure is lattice matched. This lattice matched high-quality Ge layer, as revealed by the TEM micrograph with the underlying AlAs serving as an etch stop/sacrificial layer, and can be used to demonstrate Ge based NSFETs. The thickness of the high-quality Ge layer is 80 nm, owing to the lattice matched Ge/AlAs heterointerface, which is significantly higher than conventional Si/SiGe and Ge/SiGe NSFETs thus showing potential for integration of higher number of vertically stacked virtually defect-free NSs.

4.3 Ge n- and p-NSFET structure and model calibration

This section introduces three NSFET architectures based on Ge/III-V material systems and discusses their structure, model and calibration for 0.5 V Ge CMOS operation for advanced technology nodes. **Figure 29(a)** shows the Ge FinFET structure used in Chapter 3 for Ge material model calibration and simulation, which is a starting point for this work. **Figure 29(b)** shows the NSFET A structure utilizing a high- κ dielectric stack (Si cap/SiO₂/HfO₂/Metal). NSFET B utilizes the same geometry with an alternate gate stack (GeO_x/Al₂O₃/HfO₂/Metal), where the higher dielectric constant of Al₂O₃ compared to SiO₂ is expected to provide improved electrostatic control through a higher effective oxide thickness (EOT). Strain (compressive or tensile) in p-NSFET channels is expected to improve the hole mobility [13-15] but tensile strain can prove to be more beneficial due to dominance of LH-valley over HH [16, 17]. Considering this, **Figure 29(c)** shows the NSFET C architecture, which introduces an additional In_xGa_{1-x}As layer beneath the Ge layer within the NS to act as a strain template and which will provide an epitaxial tensile strain in Ge while utilizing the same gate stack as NSFET A. **Figure 29(d)** shows the gate stack used as a

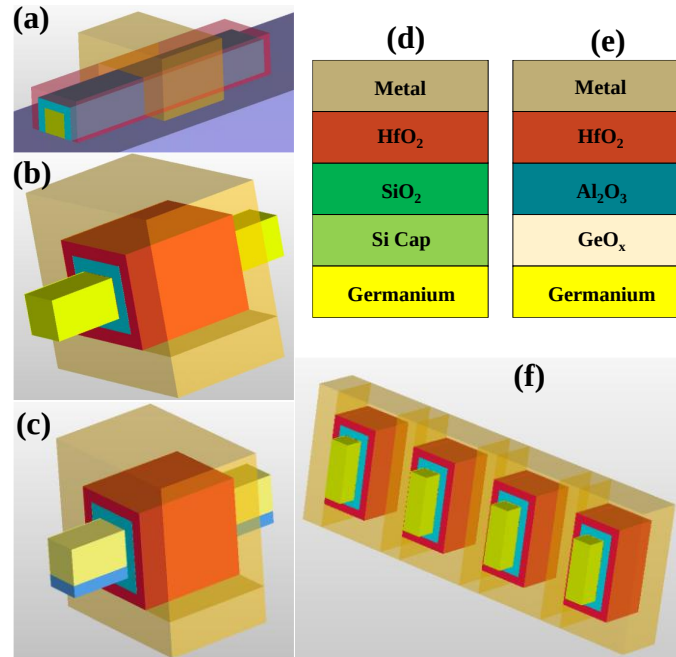


Figure 29. Schematic of (a) structure used for calibration of simulation model, (b) NSFET A and B with different gate stacks, (c) NSFET C with In_xGa_{1-x}As strain template, (d) gate architecture used in model calibration and NSFET A and C, (e) gate architecture used for NSFET B, (f) 4-layer stacked NSFET.

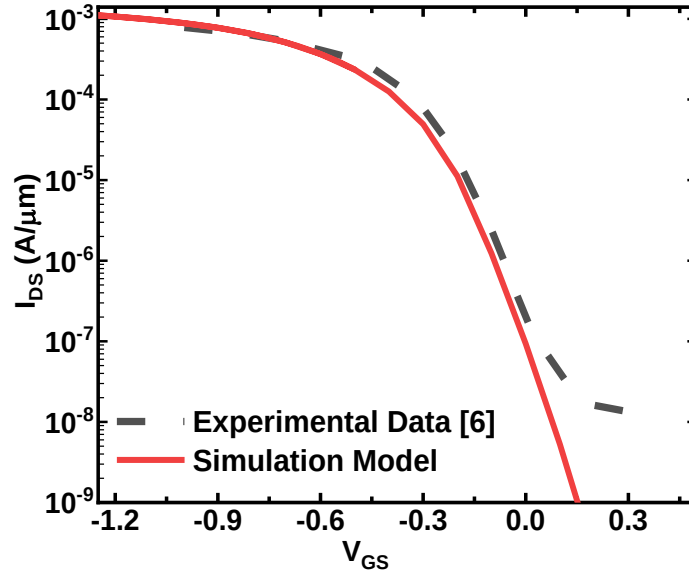


Figure 30. Model Re-validation with p-NSFET experimental data from Ref. [6].

reference to calibrate the FinFET model discussed earlier in Chapter 3, and **Figure 29(e)** shows the modified gate stack utilizing composite $\text{HfO}_2/\text{Al}_2\text{O}_3/\text{GeO}_x$ [18]. Due to the lattice matched Ge/AlAs heteroepitaxial growth, the 3D stacked NS layers (N) can be extended to any desirable number, *consequently*, **Figure 29(f)** shows the 4-layer NSFET structure. It is expected that the electrostatics and confinement effects within a FinFET and a GAA NSFET will vary considerably. **Figure 30** shows the re-validation of the simulation model for experimental Ge p-NSFET data reported in Ref. [6].

The benefits of these three NSFET architectures are studied through realistic simulations using Synopsys Sentaurus TCAD [19] considering a 3D numerical solver while accounting for the classical drift-diffusion and quantum-corrected quasi-ballistic physics. The models included here capture a multivalley band structure for Ge and InGaAs through a 6x6 k.p calculation within the simulation framework. The deformation potentials for tensile strained Ge and InGaAs are calculated in conjunction with the MLDA utility which accounts for the quantum confinement effects within the narrow channels. The band structure, band narrowing, mobility and effective mass are derived as a function of doping densities and mole-fractions. The physics invoked within the model performs geometry, band structure and effective mass dependent quantum corrections for all devices variations. A gaussian distribution of $6 \times 10^{12} \text{ cm}^{-2} \text{ eV}^{-1}$ interface trap density are included at the oxide/Ge interface to account for the unoptimized interface. Direct source-to-drain

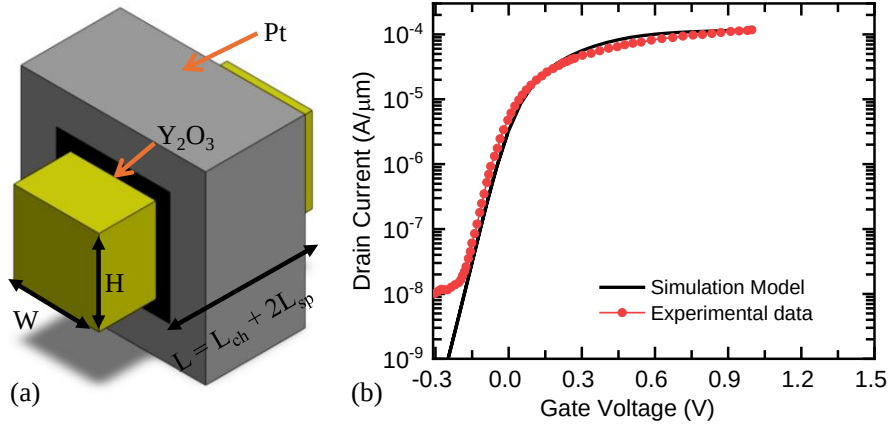


Figure 31. (a) The structure used for simulation for a single nanosheet and (b) drain current versus gate voltage characteristics for the *n*-NSFET reported in Ref. 6 and the simulation model data. Both simulated and experimental results are in agreement, which validates the model data for Ge-on-AlAs nanosheet transistor.

tunneling (SDT) based on WKB approximation has been ignored in this work as it is expected to have a negligible effect on the device performance for channel lengths above 10 nm, even though Ge has a low effective mass. In addition, the orientation of the Ge device (*i.e.*, $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$) determines the extent of SDT, where $\langle 100 \rangle$ has relatively low effect compared to other orientations.

The Ge *n*-NSFET transistor simulation model is calibrated with device data reported in Ref. 6 for a Pt/Y₂O₃/Ge-based gate stack with known material and band structure properties of Ge epitaxial layers [16] [20]. This device structure utilizes a 3 nm Y₂O₃ as high- κ gate dielectric, a boron-doped channel with a concentration of $\sim 10^{15} \text{ cm}^{-3}$, a phosphorus-doped source/drain (S/D), and an 80 nm channel length with 3 nanosheets of 90 nm wide and 40 nm thick, shown in **Figure 31(a)**. The match between the simulation model and the experimental device data is seen to be a good fit, shown in **Figure 31(b)**, thus enabling a reasonably accurate prediction for scaled devices approaching the semi-classical regime. The high- κ gate dielectrics such as Y₂O₃ and HfO₂ can enable a thicker physical thickness of the gate oxide (1 nm to 3 nm) mitigating quantum tunneling-induced gate leakage while maintaining a good scaled equivalent oxide thickness (EOT) of < 1 nm.

4.4 NSFET Process non-idealities: Impact of incomplete sacrificial layer etch

The Ge-on-AlAs NSFET device, along with a high mobility Ge channel provides a NSFET process which enables lattice matched epitaxial growth as well as superior etch selectivity between active Ge layers and the sacrificial AlAs layers is required. Further, the wet-etch (vapor etch) of the AlAs using HF/BOE can provide a much superior etch selectivity than existing Si/SiGe systems, which rely on directional dry-etch process with limited chemical selectivity. Post etching, the intermediate structure is indistinguishable from conventional Ge NSFET, except for the virtually defect-free channel. Another advantage of this system is that AlAs, by its very nature, oxidizes readily when exposed to ambient environment resulting in the formation of compositional Al-based oxides [21]. Furthermore, the AlAs has a high band offset over Ge, resulting in reduced unwanted leakage outside the Ge channel. Considering this, if any AlAs layer is un-etched during the NSFET fabrication process, it would provide minimal conduction and have reduced chances of shorting with adjacent regions. Additionally, such an un-etched AlAs residue would most likely oxidize, resulting in an even more negligible concern for device operability. On the other hand, if such an un-etched residue is a conductive material such as Si or low bandgap SiGe, it might be a major concern to device operation, yield, and reliability due to the unwanted random shorting filaments.

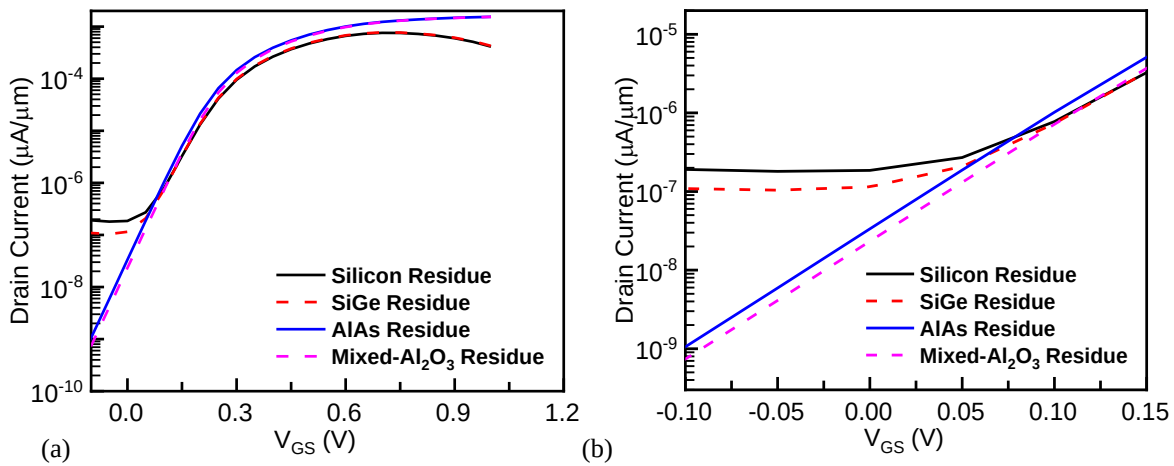


Figure 32. Impact of imperfect etching of the sacrificial layer during Ge n-NSFET fabrication resulting in residue on the simulated (a) I_{DS} versus V_{GS} characteristics of 4-channel NSFET, and (b) close-up view at the low voltage off-state impact.

A wide range of process errors/nonidealities may occur during the fabrication process for a multilayer NSFET, especially at dense ultra-scaled nodes. In the context of the sacrificial

interlayer etching process, the incomplete etch of the interlayer can result in serious degradation of the device's performance. Moreover, this residue/filament can result in an electrical short between adjacent channels and in the worst case, with the S/D. Depending on the process and the starting multilayer epitaxial stack (*i.e.*, Ge/Si epitaxy, Ge/SiGe epitaxy, and Ge/AlAs epitaxy), the interlayer residue may be composed of particles of Si, SiGe or AlAs. In the case of AlAs sacrificial layers, complete oxidation of any left-over residue is most likely resulting in an insulting residue filament. This creates 4 potential types of residues corresponding to each fabrication process flow (Ge-on-Si, Ge-on-SiGe, and Ge-on-AlAs) discussed earlier. The impact and probability of shorting increases as the number of NSs increases, a single-sheet NSFET will have no concerns of shorting. Here we analyze the impact of shorting and residues for the 4 different processes for a 4-stack NSFET device. The analysis is done using the calibrated TCAD models discussed in the previous section.

If the residue has no impact on I_{ON} and I_{OFF} compared to 4-channel NS, one can conclude that the fabrication process and device structure is robust and no impact on yield can be expected. This is the best-case scenario. For this analysis, it is assumed that the lower-most NS experiences an incomplete etch during the process leaving behind residue, while the rest of the NS channels function optimally. It is also assumed that the etchant was able to enter from both sides as is the

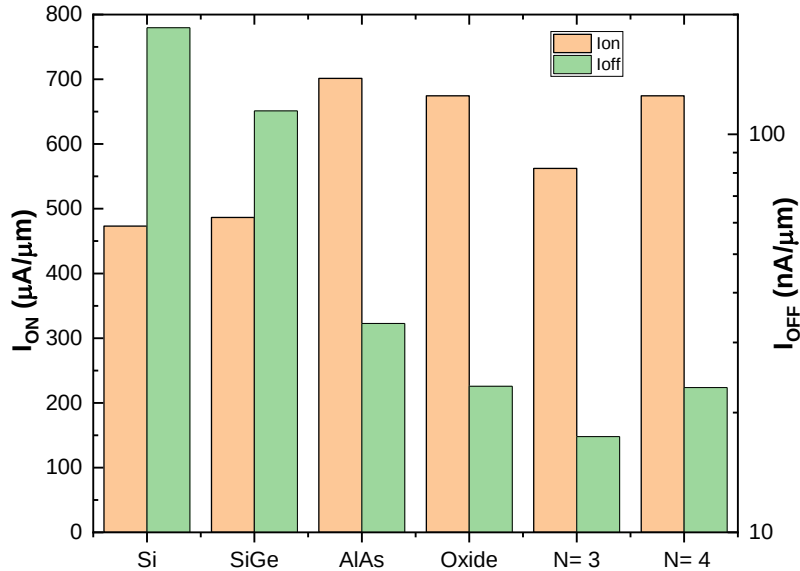


Figure 33. I_{ON} and I_{OFF} comparison of n-NSFETs with 3 and 4 channel (un-shortened) with 4 potential types of residues. The 4 NSFET data on the right should be used as a reference to compare the relative impacts of the different residues.

case with most isotropic wet/vapor processes, but the central region of the sacrificial layer remained unexposed, consequently forming the residue which is a thin filament near the center of the nanosheet. **Figure 32** shows the impact of imperfect etching of the sacrificial layer during NSFET fabrication resulting in residue on the simulated I_{DS} versus V_{GS} characteristics of 4-channel NSFET. It is evident that the I_{OFF} current drastically rises due to the short between the channels for the Si and SiGe residue case, compared to the AlAs case or the case where the residue is a mixture of Al and As oxides. **Figure 33** compares simulated I_{ON} and I_{OFF} for the 4 potential types of residue cases with un-shortened NS of 3 and 4. In the case of AlAs unetched residue during the Ge-on-AlAs NSFET fabrication process, I_{ON} and I_{OFF} remain unaffected and comparable with the 4-layer nanosheet. Between the AlAs and oxide residue case, as expected the oxide exhibits more resilience due to an increased insulation provides by the oxide. It indicates that the Ge-on-AlAs NSFET fabrication process has a large degree of immunity to process variations compared with the Si or SiGe case, resulting in potentially improved yield and reliability.

4.5 Ge NSFET & Ge FinFET: A brief comparison

Prior to investigating the performance of advanced NSFETs, it is crucial to highlight the region of operation where NSFETs can out-perform FinFETs. In other words, it is crucial to understand in a qualitative and quantitative way, why one should go for NSFET devices which have a higher process complexity (as seen in previous sections) over FinFETs. **Figure 34** shows that moving to a Ge based GAA/nanosheet/quad-gate architecture from a tri-gate/FinFET architecture for fixed dimensions (N5 node) as well as gate stack can provide a significant boost in I_{ON} (12 %), I_{ON}/I_{OFF} ratio (5.3 $\times$) as well as SS (9.5 %). The calibrated model is extended to an undoped channel and a work function of 4.4 eV in order to tune the V_{TH} (~ 0.1 V) to operate optimally for 0.5 V CMOS. **Figure 35** provides an insight into the dependence of device performance of the Ge FinFET, NSFET A, B and C on the channel aspect ratio (AR). Note that the performance is evaluated for fractional (*sheet-like*) and integer (*fin-like*) ARs. Due to the higher inversion charge density attributed to the GAA architecture, the NSFET devices show higher I_{ON} for almost all ARs, this is evident through the on-state inversion charge distribution shown in **Figure 36**. The approximate charge densities associated with the contours have been highlighted to emphasize the subtle difference between the charge density distribution, and correspondingly, a marginal difference in I_{ON} can be seen in **Figure 35(a)** between the NSFET and the FinFET. Due

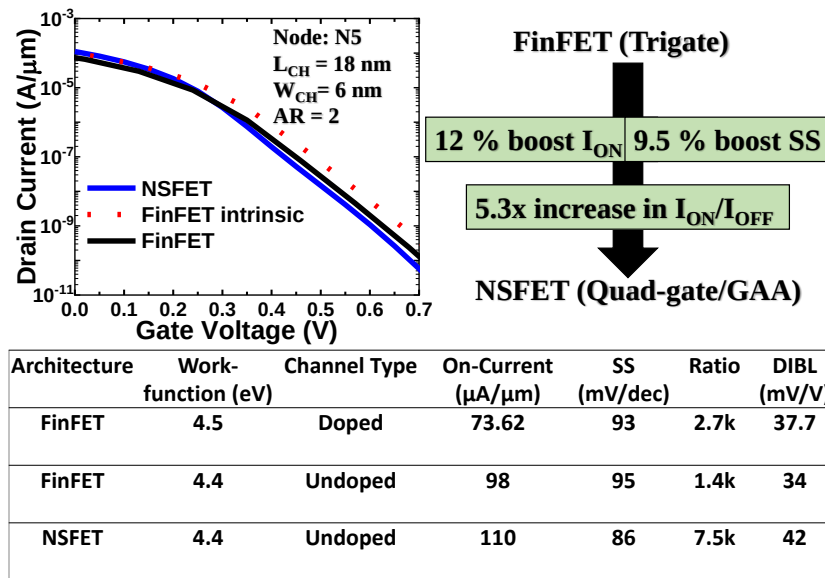


Figure 34. Transition in device architecture from Ge p-FinFET to p-NSFET resulting in performance improvement (I_{ON} , I_{ON}/I_{OFF} ratio and SS) at the N5 node.

to rise in hole mobility by tensile strain in ϵ -Ge, the NSFET C shows significant rise in I_{ON} for increasing In composition. The bandgap of the Ge channel reduces with strain resulting in higher leakage as can be seen through degrading I_{ON}/I_{OFF} ratio for the strained NSFET C (see **Figure 35b**). In addition, strain is seen to slow down the degradation of SS for higher AR (see **Figure 35c**). Measures must be taken for the strain relaxation in nanoscale devices as relaxation could occur during source and drain processing as well as lithography steps. Since, it could negate the benefits of the strain induced device performance enhancement. In terms of electrostatic control, the NSFET B shows the optimal SS, I_{ON}/I_{OFF} ratio, and DIBL. All the metrics for the FinFET architecture remain approximately independent of AR (see dotted lines in **Figure 35** for all device metrics), whereas the performance of the NSFET is AR sensitive (see solid lines in **Figure 35** for all device metrics). The SS of the NSFET is superior to the FinFET for nearly all AR owing to the

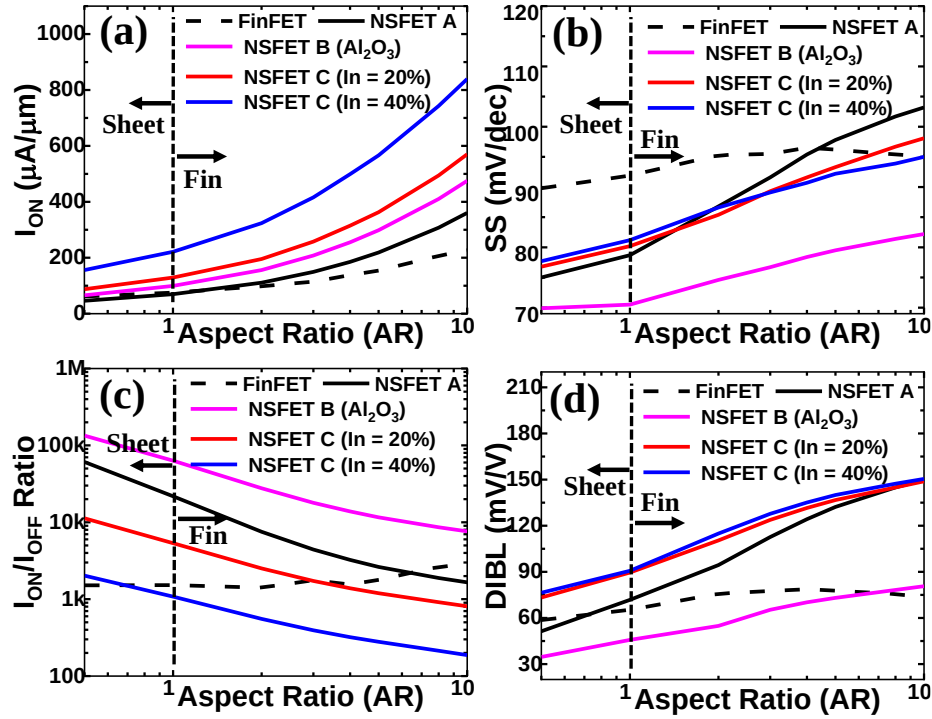


Figure 35. The dependence of device metrics (a) I_{ON} , (b) I_{ON}/I_{OFF} ratio, (c) SS and (d) DIBL on channel AR for fixed W, indicating a superior performance for NSFET compared to FinFET for nearly all aspect ratios at the N5 node.

GAA architecture resulting in better electrostatic control. This difference in the performance trends with AR for the NSFET and FinFET is due to the difference in electric field distribution, which affects the depletion and inversion charge densities in the channel and can be used to understand

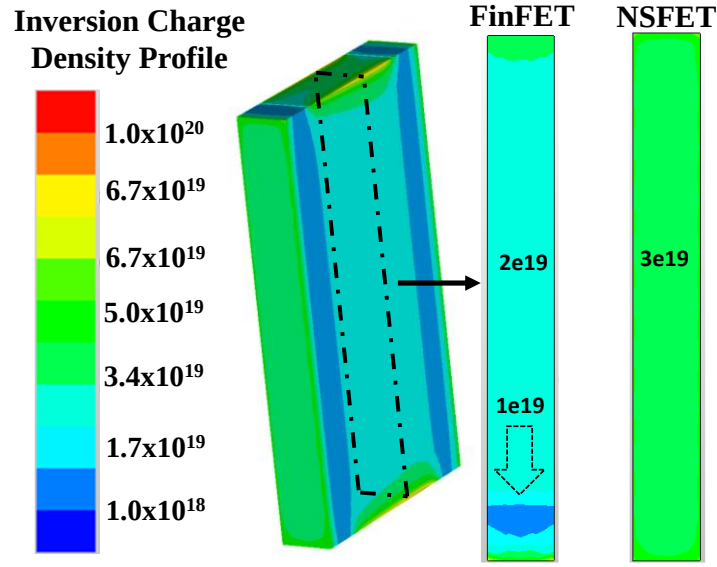


Figure 36. Difference in on-state inversion charge density distribution between NSFET and FinFET of identical dimensions resulting in a difference in I_{ON} .

the performance trends shown in **Figure 35**. The SS and I_{ON}/I_{OFF} ratio can be inferred from the carrier density in the off-state at 0.5 V. A smaller off-state carrier density in the channel indicates a lower leakage current and correspondingly, a higher I_{ON}/I_{OFF} ratio and low SS. In order to explain these behaviors, the off-state charge density of NSFET and FinFET for identical dimensions as a function of AR is shown in **Figure 37**. For $V_{DS} = 0.5$ V and $V_{GS} = 0$ V, the charge density distribution can be seen as a function of AR and device architecture. The charge density is chosen as the indicator of device behavior as it captures the cumulative effect of all self-consistent physical phenomena within the device, and it directly affects the current flowing through the device thus showing direct correlation with device performance. For fractional AR in **Figure 35** and **Figure 37**, due to the strong control over the entire volume of the channel provided by the 4 gates in the NSFET, the leakage charge densities are very small. This indicates that the leakage in this device will be low and the device now provides a much higher I_{ON}/I_{OFF} ratio at the voltage range of 0.5 V, indicating improved SS. This was possible due to the superior control on the charges in short and narrow channel devices. As one transitions to the FinFET architecture, the lower gate is removed and hence the control on the charges only reduces marginally. This can be seen through the rise in off-state charges in the FinFET compared to the NSFET, seen in **Figure 37**.

In **Figure 37**, the charge density contours are symmetric in all 3-directions for the NSFET, whereas they are skewed in the vertical direction for the FinFET. This is expected as the charge

densities follow the electric field contours which are determined by the geometry and the number of gates. Depending on the AR of these quantum confined device architectures, the channel could be nearly or completely volume inverted, and the charge conduction occurs primarily in the center of the channel. Thus, the charge densities at the center of the cross-section in **Figure 37** are a good metric to understand the behavior of the device. For low leakage (*i.e.*, low SS and high I_{ON}/I_{OFF} ratio), the approximate charge density at this central point should be as low as possible. Due to the asymmetric electric field in the FinFET, the charges re-distribute in such a way that the central conducting portion remains at low density and the charges migrate to other portions of the fin (*see Figure 37* lower left *green contour*). On the other hand, the NSFET has a symmetric charge profile and the charges are forced to re-distribute accordingly and this results in a relatively higher off-state charge density at the center for higher AR. In essence, for higher AR, as both the FinFET and

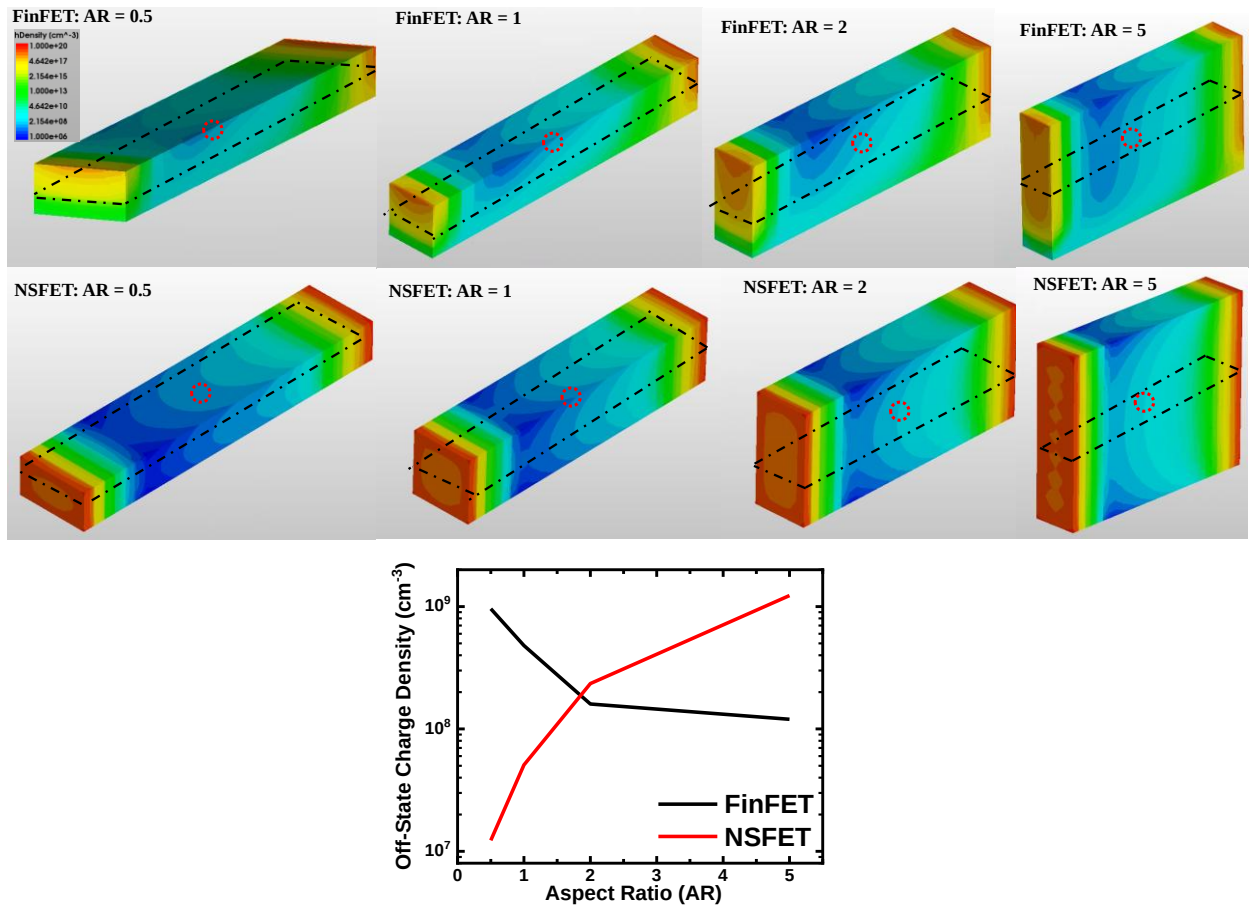


Figure 37. Effect of AR on the off-state charge density of NSFET and FinFET for identical dimensions (*i.e.*, W and L) with AR varying from 0.5 to 5. This off-state leakage charge is probed at the central cross-section and shown as a function of AR for the FinFET and NSFET.

NSFET begin to lose control over the volume of the charges in the channel (*i.e.*, increase in SS and decrease in I_{ON}/I_{OFF} ratio), the ability to re-distribute the charges in an asymmetric manner proves to be the differentiating factor and benefits the FinFET performance to a certain extent. For AR beyond 2, the asymmetric charge distribution in the FinFET allows the central charge density to remain relatively constant compared to the NSFET, this off-state charge density variation is shown in **Figure 37** (right). The DIBL dependence on AR for a fixed W can be inferred from the SS variation to follow a similar trend, as both these quantities are measures of the electrostatic integrity of the channel which is a function of the device architecture and geometry. Thus, to take complete advantage of the NSFET architecture, sheet-stacking should be the design pathway rather than AR scaling as discussed in the following sections. For the range of AR studied in this work, the NSFET is superior to the FinFET in nearly all aspects, except in the scenarios where, (i) ease of processing and yield are prioritized over performance, (ii) ease of design due to AR independent metrics, and (iii) DIBL is the design priority. For further study below, we use NSFET B, as it shows optimum performance with a feasible gate stack.

4.6 Ge NSFET n- and p-device Performance & Benchmarking

The 4-fold improvement in device performance provided by NSFET over FinFET seen in this section (see **Figure 34** and **Figure 35**) was possible with maximum re-utilization of existing FinFET processing and design capabilities, thus justifying further device and circuit investigations at ultra-scaled nodes [1] at 0.5 V CMOS.

The advanced GAA nodes have three flavors (HP, HD and SRAM) associated with each node N2.1, N1.5, N1 and N0.7 for application specific design consideration. **Figure 38** shows the performance of the proposed Ge/AlAs NSFET B architecture for dimensions corresponding to the advanced nodes and the three flavors as a function of number of stacked NS layers (N). The I_{DS} - V_G characteristics for the high-performance (HP) flavor (wider NS) of the nodes is shown in

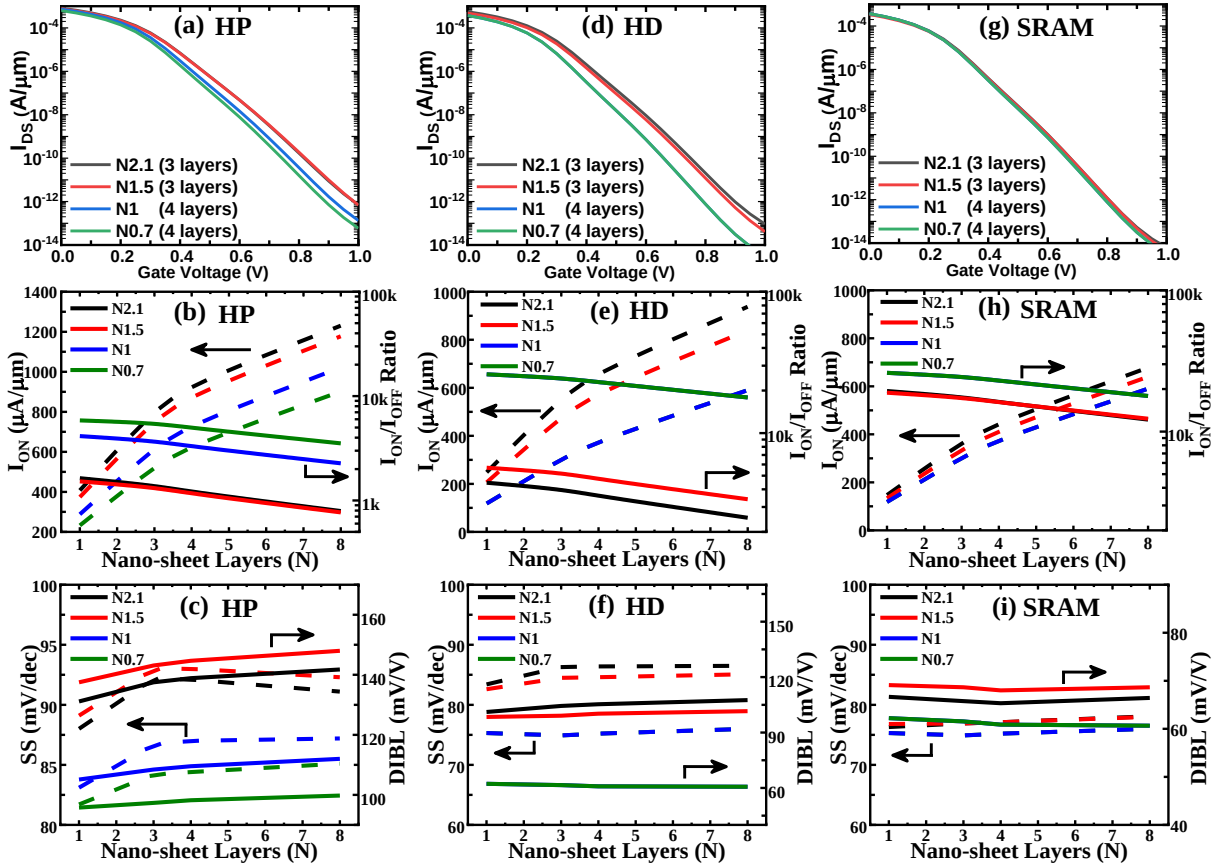


Figure 38. Proposed Ge NSFET B device metrics at advanced nodes N2.1, N1.5, N1 and N0.7 are shown; (a) I_{DS} - V_G , (b) I_{ON} and I_{ON}/I_{OFF} ratio, (c) SS and DIBL for the HP flavor; (d) I_{DS} - V_G , (e) I_{ON} and I_{ON}/I_{OFF} ratio, (f) SS and DIBL for the HD flavor; (d) I_{DS} - V_G , (e) I_{ON} and I_{ON}/I_{OFF} ratio, (f) SS and DIBL for the HD flavor; (g) I_{DS} - V_G , (h) I_{ON} and I_{ON}/I_{OFF} ratio, (i) SS and DIBL for the SRAM flavor. Table I shows the corresponding dimensions for the nodes.

Figure 38(a). The I_{ON} is expected to rise linearly with N due to added parallel conduction paths, but as shown in **Figure 38(b)** (see dotted lines), this rate of increase of I_{ON} is sub-linear, and this can be attributed to the increase in self-loading due to rise in parasitic capacitance [22]. Thus, the benefit of improved I_{ON} provided by layer stacking diminishes at higher N . Further, among the four nanoscale nodes, the drive strength drops for lower nodes due to narrower channel widths. The I_{ON}/I_{OFF} ratio (*i.e.*, leakage) drops steadily with N as shown in **Figure 38(b)** (see solid lines) and the lower nodes provide lowest I_{OFF} as indicated by the high I_{ON}/I_{OFF} ratio. The SS in **Figure 38(c)** (see dotted lines) can be seen to degrade slightly for higher N , whereas DIBL in **Figure 38(c)** (see solid lines) is nearly constant for all N . Furthermore, the lower nodes provided a superior SS indicating an improved electrostatic control over the channel owing to the narrower widths. The $I_{DS}-V_G$ for the high density (HD) flavor (moderately wide NS) of the nodes is shown in **Figure 38(d)**. A trend similar to the HP nodes can be seen for the I_{ON} and I_{ON}/I_{OFF} ratio as shown in **Figure 38(e)**. The absolute values of I_{ON} have decreased (due to reduced width) and the I_{ON}/I_{OFF} ratio has increased (better control over the channel due to increased confinement attributed to narrower width) compared to the HP nodes. The variation of SS and DIBL (as shown in **Figure 38f**) with N is further suppressed for the HD nodes compared to the HP nodes. This suppression is also followed by a reduction in absolute values of SS and DIBL, owing to the superior electrostatic control provided by the narrow width, resulting in increased quantum confinement in the channel.

TABLE I

Benchmarking of lattice matched Ge/AlAs and pseudomorphic Ge/InGaAs p-NSFETs with reported GAA p-FETs. The proposed NSFET A, B and C shows excellent low power performance and comparable drive capabilities at reduced footprint.

Ref.	Material	Architecture (<i>p</i> -FET)	L (nm)	W [or D] (nm)	H [or D] (nm)	No. of sheets [or wire]	I _{ON} ($\mu\text{A}/\mu\text{m}$)	I _{ON} /I _{OFF}	SS (mV/dec)	Supply (V)
[6] and [38]	Ge	NSFET	90	80	40	3	1650	10^4	130	1
	Ge	NSFET	90	80	40	1	717	10^5	105	1
[4]	Si	NSFET	45	30	8	7	3000	10^6	64	1
[28]	ϵ -Ge	Nanowire	45	13	13	1	500	10^3	75	0.5
[39]	GeSn	GAA	40	20	5	3	58	—	110	0.5
[31]	SiGe	NSFET	25	100	5	1	508	5×10^3	79	0.5
	SiGe	NSFET	55	100	5	1	300	3×10^3	67	0.5
[31]	GeSn	NSFET	90	30	2.4	8	170	1.6×10^7	64	0.5
[32]	GeSn	NSFET	120	87	12	4	42	2×10^4	89	0.5
[33]	Ge	Nanowire	40	9	9	2	524	5.24×10^3	81	0.5
<i>This work (N5)</i>										
NSFET A	Ge	NSFET	18	6	6	1	69	2.18×10^4	78	0.5
NSFET B	Ge	NSFET	18	6	6	1	99	6.32×10^4	70	0.5
NSFET C20	ϵ -Ge	NSFET	18	6	6	1	129	5.34×10^3	80	0.5
NSFET C40	ϵ -Ge	NSFET	18	6	6	1	221	1.07×10^3	81.2	0.5

The I_{DS} - V_G for the SRAM flavor (narrow NS) of the nodes is shown in **Figure 38(g)**. Due to further reduction in channel width, these devices have increased quantum confinement resulting in improved I_{ON}/I_{OFF} ratio and a diminished I_{ON} (**Figure 38h**). In addition, the SS and DIBL are improved further compared to the HP and HD nodes as seen in **Figure 38(i)**. The effect of quantum confinement on the device performance for narrow NSFET is discussed below.

The quantum confinement of carriers near the oxide/Ge interface results in a shift in the charge centroid away from the interface and changes the conduction properties near the interface. In low bandgap materials such as Ge, one important problem in having functional and normally-off transistor is the low V_{TH} . As the V_{TH} becomes lower (or tends to normally-on operation), the controllability in terms of the ability of the gate to modulate the charges in the channel reduces. This can be seen from the sharp fall in I_{ON}/I_{OFF} ratio, as seen in **Figure 38**. As the width becomes narrower, the charge centroid shifts away from the interface due to quantum confinement followed by a slight increase in V_{TH} [23, 24]. This results in a slight reduction in on-current as well as decrease in effective oxide capacitance. In ultra-scaled devices, with increasingly narrower channels, this V_{TH} boost (and corresponding increase in I_{ON}/I_{OFF} ratio and decrease in SS [24]) can become a valuable improvement in low bandgap-based transistors. We refer to this increase in V_{TH} and I_{ON}/I_{OFF} ratio as improved electrostatic control. There have been experimental and theoretical reports related to this QC effect [23-27]. Furthermore, the pushing of the charges away from the interface will improve the performance of real devices due to reduced semiconductor-oxide interface scattering, and such a boost could prove beneficial for scaled multi-gate devices. Due to identical dimensions as well as number of stacked layers in the N1 (green) and N0.7 (blue) HD

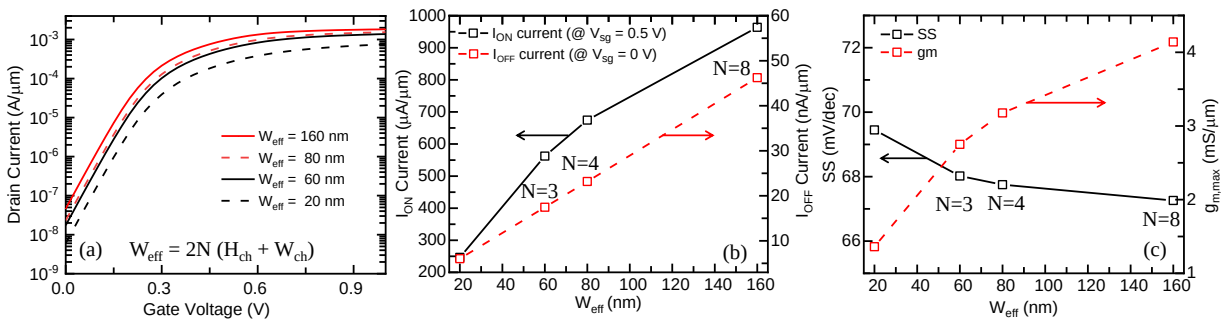


Figure 39. The impact of N scaling on (a) drain current versus gate voltage, (b) I_{ON} and I_{OFF} , and (c) SS and maximum transconductance. Scaling the number of nanosheets N enables a proportionate scaling of the effective width for the Ge n -NSFET.

and SRAM flavors, the device metric data for the NSFET B in **Figure 38(e-f)** and **Figure 38(h-i)** are colinear. The following discussion focuses on the Ge based n-NSFET to draw different insights into this system. These Ge/AlAs and Ge/InGaAs NSFET designs are benchmarked with recent experimental reports of Ge, SiGe, GeSn and Si based p-GAA devices in **Table I** [7], [6], [28]-[33].

The Ge-on-AlAs *n*-NSFET performance can be scaled using the number of nanosheets (N) in the stack as well as the width (W) and height (H) of the individual nanosheet. The N scaling is a preferable choice for boosting the ON current (I_{ON}) when the area constraint on the device design is stringent. The NSFET structure is surrounded by the gate on all four sides, and consequently, the effective width (W_{eff}) for this multi-gate transistor can be defined as $W_{eff} = 2N(W + H)$. Scaling N from 1 to 8 will consequently result in a larger W_{eff} , and the effect on the drain current *versus* gate voltage (I_D - V_{GS}) (see, **Figure 39a**) can be seen as a rise in I_{ON} as well as the OFF current (I_{OFF}) (see, **Figure 39b**). The shape of the I_D - V_{GS} can be seen to remain similar as N is increased indicating similar electrostatics and subthreshold slope (SS), as shown in **Figure 39(c)**. The maximum transconductance ($g_{m,max}$) (see, **Figure 39c**) rises substantially as I_{ON} is increased. The rate of rise of I_{OFF} is linear due to the additional resistive paths for leakage conduction (see **Figure 40**). Interestingly, the rate of rise of I_{ON} decreases as the number of nanosheet layers increases and the trend is sub-linear. This is due to the parasitic resistances forming a ladder network resulting in an unequal current flowing through each nanosheet. The parasitic resistance

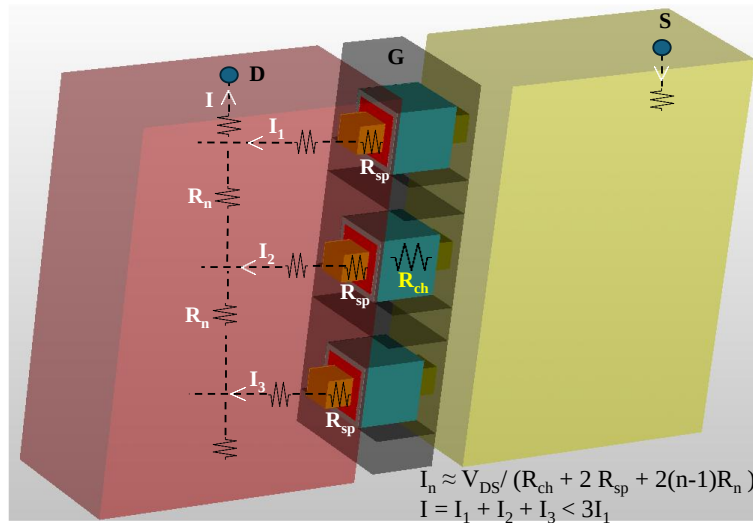


Figure 40. Parasitic resistance network is schematically represented using lumped parameters. Different resistance and current paths are indicated. The approximate current in the *n*th NS is shown.

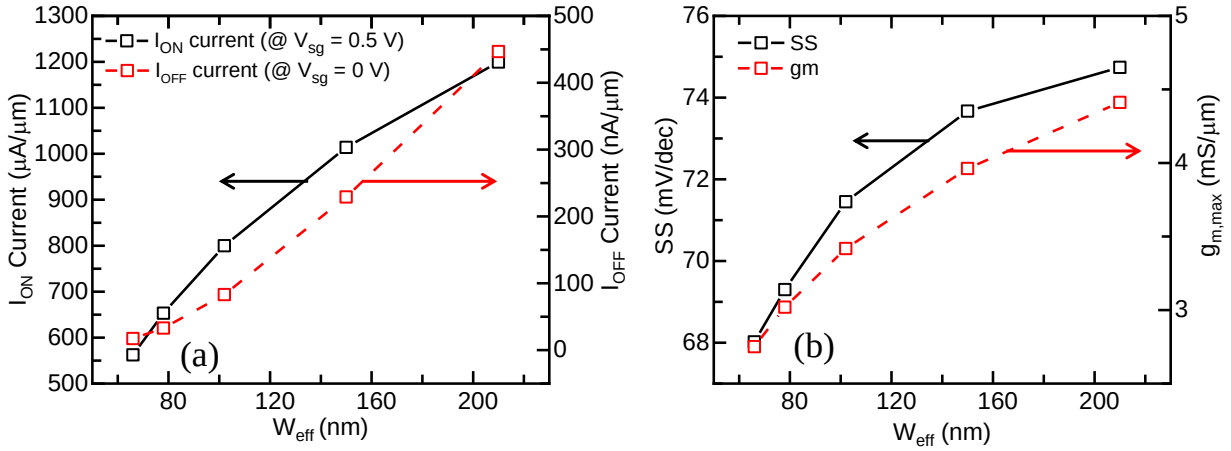


Figure 41. The impact of W scaling on, (a) on-current and off-current and (b) SS and maximum transconductance. Wider nanosheets can provide better drive strength at the cost of higher SS.

ladder network is schematically represented using lumped parameters, as shown in **Figure 40**. One can find from this figure that one NS will conduct the maximum current, here I_1 , while each subsequent NS channel will conduct a smaller current as shown by the equation below, resulting in eventual saturation. The approximate equation for the current through the n^{th} nanosheet in a stack of N layers is shown in **Figure 40**, where, I_1 , I_2 , and I_3 are I_{ON} current in each NS channel, and R_{ch} , R_{sp} , and R_n are resistances in channel, spacer, and drain region, respectively. The degradation of current conduction suggests that while additional layers continue to improve I_{ON} , the extent of these improvements decreases with each subsequent layer due to an increase in parasitics. Similarly, SS and $g_{m,max}$ demonstrate a degradation with increasing NS layers (see, **Figure 39c**). For example, with increased NS layers from 1 to 4, the $g_{m,max}$ improved by $\sim 170\%$ compared to the improvement in $g_{m,max}$ from 4 to 8 layers of only $\sim 30\%$. Thus, with sufficient NS layers, improvements in all three trends (I_{ON} , SS, and $g_{m,max}$) will eventually saturate.

If the drive strength is to be improved, even at the cost of the device area, the width scaling of the NS is an alternative approach. The impact of wider widths (5 nm to 30 nm) on the performance of a 3 NS device is shown in **Figure 41**. The I_{ON} and I_{OFF} scale up with increasing W due to a wider conductive path for the channel current as shown in **Figure 41(a)**. Beyond 3 NS, if the primary design concern is large I_{ON} for the same W_{eff} then the width scaling proves to be a

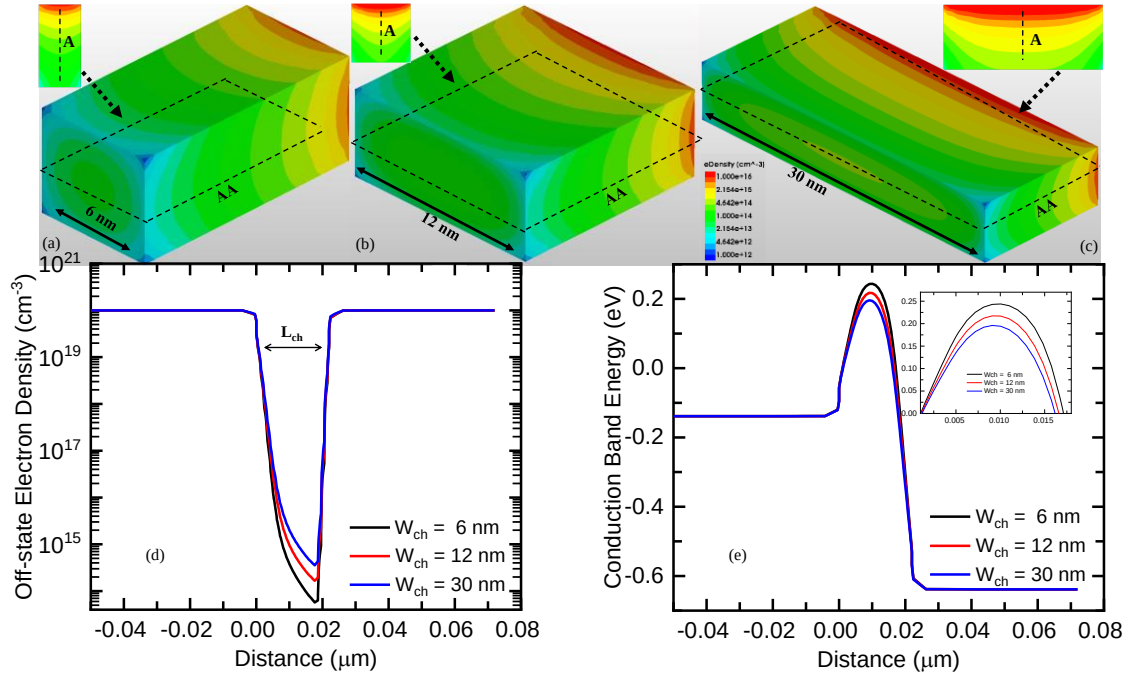


Figure 42. (a)-(c) Electrostatic potential variation across the channel in 3D geometry, and (d-e) the off-state electron density across the central cross section of the nanosheet channel.

better alternative over the number of NS due to reduced parasitic resistances. Similarly, the $g_{m,max}$ also increases with wider channels as shown in **Figure 41(b)**. The SS rises for wider NSs due to

Table II

Benchmarking of this work with other relevant nanosheet n-FETs and gate all-around FETs

Ref	Material	Architecture [nFET]	L (nm)	W [or D] (nm)	H [or D] (nm)	No. of sheets [or wire, fin]	I _{ON} (μA/um)	I _{ON} /I _{OFF}	SS (mV/dec)	Supply (V)
[6]	Ge on Si	NSFET	180	90	40	3	100	10×10 ³	140	0.5
[34]	Si	GAA	5	3	19	1	421	48×10 ³	99	0.6
[34]	Si	GAA	5	3	7	2	273	⁷⁹ ×10 ³	91	0.6
[22]	Si	NSFET	10	10	5	2	30	-	80	0.65
[28]	SiGe	NSFET	45	30	8	7	3000	1×10 ⁶	64	1
[35]	Ge	FinFET	200	30	80	1	200	33×10 ⁴	72	1
[36]	Ge	NW	100	10	10	7	110	1×10 ³	68	1
This work	Ge	NSFET	12	6	5	3	562	32×10 ³	68	0.5
	Ge	NSFET	12	6	5	8	964	20×10 ³	67	0.5

the reducing electrostatic control over the channel resulting in a degrading I_{OFF} , as shown in **Figure 41(b)**. The cause of this SS degradation can be understood through the channel electron density contours in the off-state, which is a consequence of the electrostatic potential variation across the channel 3D geometry, shown in **Figure 42**. In the off-state, the electron density across the central cross-section of the NS channel should be as low as possible as shown in **Figure 42(a), (b)** and **(c)** for $W = 6$ nm, 12 nm, and 30 nm, respectively. The electron density in the wider NSs is higher (see, **Figure 42d**) due to the lower conduction band barrier energy seen by the electrons in the off state as shown in **Figure 42(e)**. **Table II** benchmarks this work alongside several other relevant n-NSFETs and GAA n-FETs.

4.7 CMOS Circuit tradeoff considerations: Multiplier, ADP and N

The effective width of multi-gate FinFETs and NSFETs determines the performance metrics and the chip area consumed by the device. Here, we define an indicator to estimate the footprint of the device, $fp = W_{CH} \times L_{CH}$. Also, the effective channel width (W_{eff}) is defined as $W_{eff} = 2N \times (H_{CH} + W_{CH})$ [27]. The dimensions of the NSFET, *here*, are chosen corresponding to the N0.7 node ($L_{CH} = 12$ nm) and the H_{CH} (5 and 14 nm) and W_{CH} (15 and 6 nm) such that W_{eff} remains fixed for a given value of N . For a fixed W_{eff} , the I_{ON} remains constant with reduction of W_{CH} , whereas the I_{ON}/I_{OFF} ratio decreases by ~ 50 % and the SS and DIBL degrade as seen in **Figure 43(a) and (b)**, respectively. This implies that, to obtain the same I_{ON} for a smaller device footprint (*i.e.*, reduction in W_{CH}) one must upscale the H_{CH} proportionately, a trend similar to the FinFET, but at the cost of electrostatic control through degrading I_{ON}/I_{OFF} ratio, SS and DIBL. This indicates that for a fixed W_{eff} , wider devices will provide better electrostatic control than thicker devices, further affirming the observation that narrower width (*e.g.*, SRAM *versus* HP flavor)

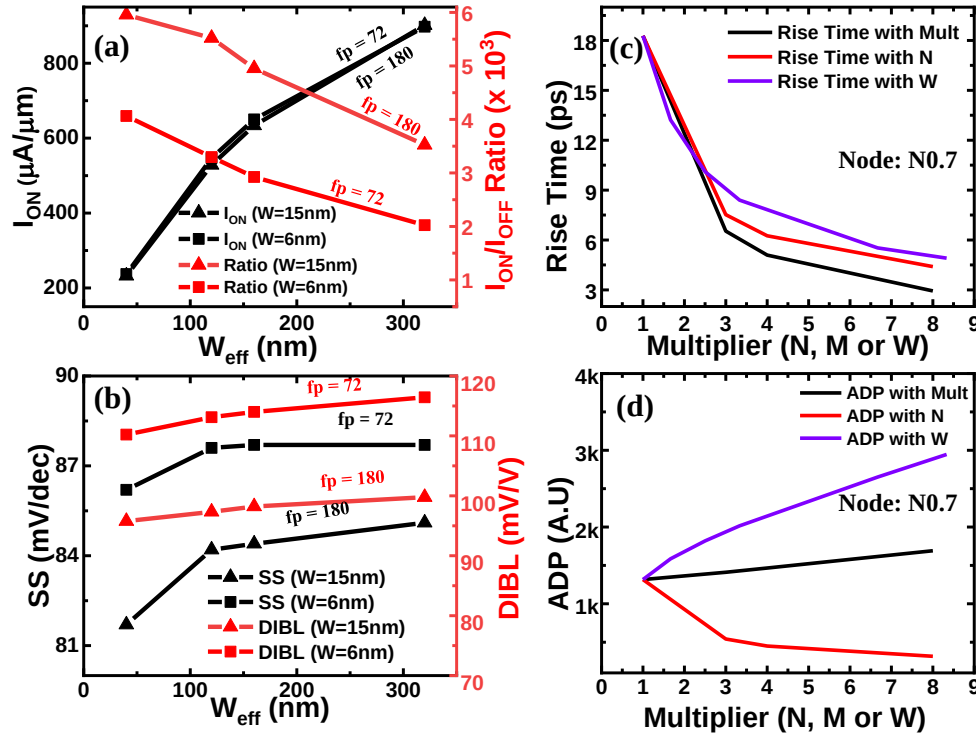


Figure 43. Iso-footprint analysis of NSFET B at N0.7 for $N = 1, 3, 4$ and 8 with (a) I_{ON} and I_{ON}/I_{OFF} ratio, (b) SS and DIBL. The estimated fp is 180 and 72 for $W = 15$ nm and $W = 6$ nm respectively. Comparison of design pathways (N , M and W) through transient circuit simulations at N0.7 (c) rise time and (d) ADP.

results in improving electrostatic control as seen **Figure 38**. For a fixed W_{CH} and H_{CH} , the 3D stacking of NS layers will increase the W_{eff} without degrading device performance. With increasing N , the W_{eff} increases resulting in metrics which are *iso-footprint*. **Figure 43(a)** shows that for a fixed footprint, the W_{eff} can be scaled using N resulting in a considerable rise in I_{ON} ($\sim 500\%$) despite the rising parasitics as discussed earlier, with an acceptable degradation in I_{ON}/I_{OFF} ratio ($\sim 50\%$). Furthermore, for a fixed footprint, the SS and DIBL remain nearly constant (**Figure 43b**) with increase in W_{eff} , establishing that increasing N is the most optimum pathway to improve device performance.

Although, the device metrics like I_{ON} , I_{OFF} , I_{ON}/I_{OFF} ratio, SS and DIBL provide an excellent means to characterize the performance of a CMOS device at scaled geometries and supply voltages, a more rigorous estimate can be obtained from transient circuit analysis. Transient circuit simulations can provide feedback regarding the cumulative effect of all the dc metrics discussed above, while driving a realistic capacitive load. Here, we use the Ge p-NSFET DUT as the pull-up network to drive a large capacitive load. The three design pathways to boost the drive strength of the NSFET DUT are, (i) use of parallel devices or mults (M), (ii) use of wider channel (W), and (iii) use of stacked layers in the NSFET or N . The unit device (*i.e.*, $M = N = W = 1$) is assumed to have dimensions corresponding to the N0.7 SRAM node, with $W_{CH} = 6$ nm, $L_{CH} = 12$ nm and $H_{CH} = 5$ nm. To study the effect of parallel devices or mults, the multiplier M is defined as the number of devices in parallel, whereas N is the number of stacked NS layers as described earlier. The width W_{CH} is defined *here* as $W_{CH} = W \times 6$ nm. The time needed to charge the capacitive load from 0 – 90 % is used as a metric to define the rise time. The transient circuit simulations assume identical source, drain and interconnect configuration for the three designs. The structures are designed such that the interconnect, source, drain and dielectrics scale proportionately as one varies device parameters such as N , M , W , H_{CH} , W_{CH} and L_{CH} , thus ensuring accurate numerical estimates of device parasitics. In addition to this physics-based parasitic estimation, the calibrated model used here assigns an additional SPICE-style resistance of 100 Ω , at each electrode to account for external factors. The choice of design pathway (N , M or W) has a distinct impact on the parasitic capacitance of the DUT as well as the footprint.

Furthermore, the device metrics (SS, DIBL, I_{ON} and V_{TH}) vary considerably due to changes in N , M or W , and the cumulative effect of these are studied through transient circuit simulations and quantified using the rise time delay (**Figure 43c**) and the area-delay-product (ADP). The ADP

is defined as the product of the rise time delay and the footprint (fp), $ADP = fp \times \text{rise time}$, as shown in **Figure 43(d)**. The rise time is nearly equal for the three pathways up to a multiplier of ~ 2 as seen in **Figure 43(c)**, beyond this, to achieve faster DUT operation (*i.e.*, lower rise time) NS stacking through higher N and device mults through higher M are superior techniques over width scaling through W. For higher multipliers beyond 3, using mults M provides better load driving capability at the cost of immense penalty on chip area. Thus, the ADP is a better metric to provide an estimate of relative merits of the three pathways. The NS stacking through higher N is the most efficient method to improve the drive strength of the DUT with minimal footprint penalty, whereas width scaling is the least efficient as seen in **Figure 43(d)**. Furthermore, the width scaling pathway proves to be challenging in terms of circuit design as the device parameters such as V_{TH} , SS, DIBL vary significantly with W, unlike M or N. The stacking of NS layers N beyond 4 is a serious challenge in traditional Si NSFETs with Si/Si_{0.7}Ge_{0.3} pseudomorphic multilayer stacks or Ge NSFETs with Ge/Si_{0.3}Ge_{0.7} or Ge/Si multilayer stacks, thus limiting the drive capability of these CMOS devices for high performance applications. This Ge/AlAs lattice-matched NSFET configuration can provide the necessary material properties (high mobility and defect-free active channel) to enable stacking N beyond 4.

4.8 CMOS Circuit Performance: Inverter and 6-T SRAM cell

This work explores a system that provides lattice matched Ge/AlAs NS multilayer epitaxial growth, which can allow performance improvement through all the pathways discussed above as well as performance improvement over existing FinFETs. In addition, we show that vertical stacking of Ge NS is the most area and delay efficient pathway for improving CMOS circuit performance at advanced nodes such as the N0.7 node. CMOS inverters are the building blocks of

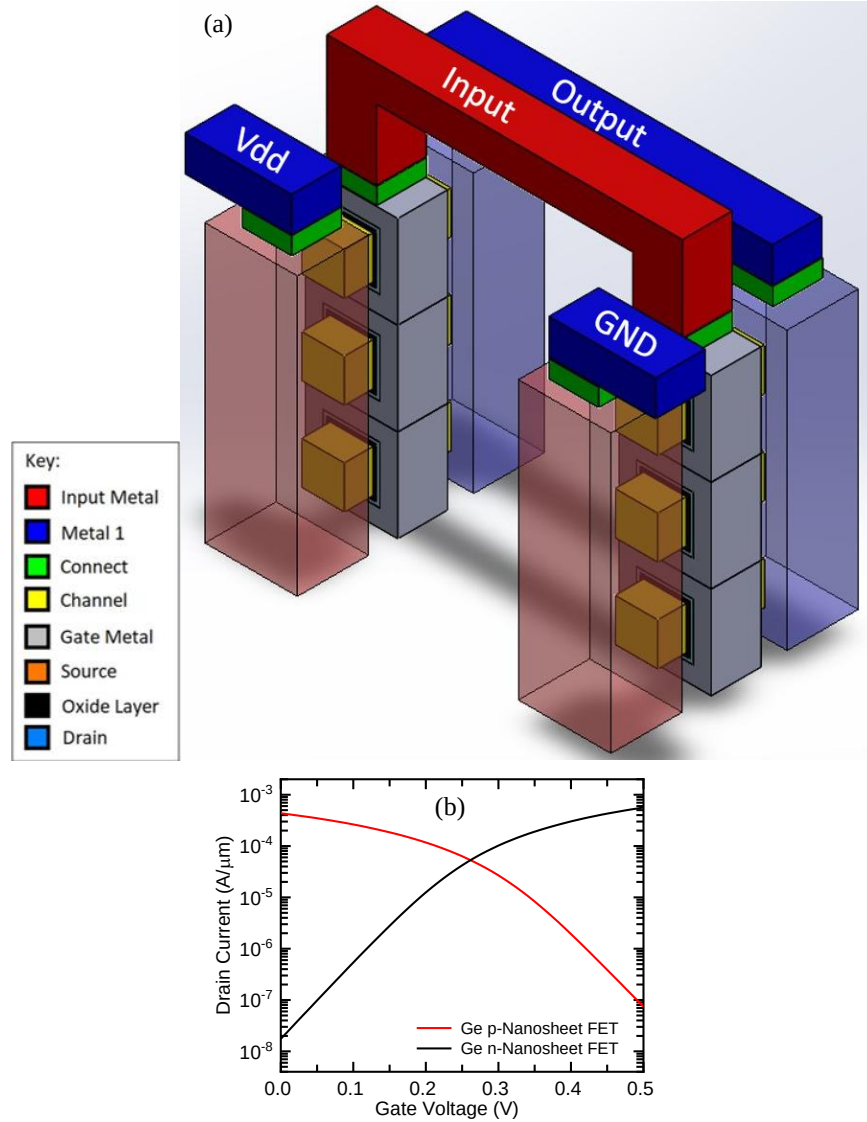


Figure 44. (a) 3D representation of the Ge-on-AlAs based NSFET-based CMOS inverter structure, and (b) drain current versus gate voltage characteristics of the same.

all digital logic, and millions are used in modern electronics. Thus, it is important to analyze and show the performance of the proposed Ge-based NSFET inverters. For an optimal inverter, both

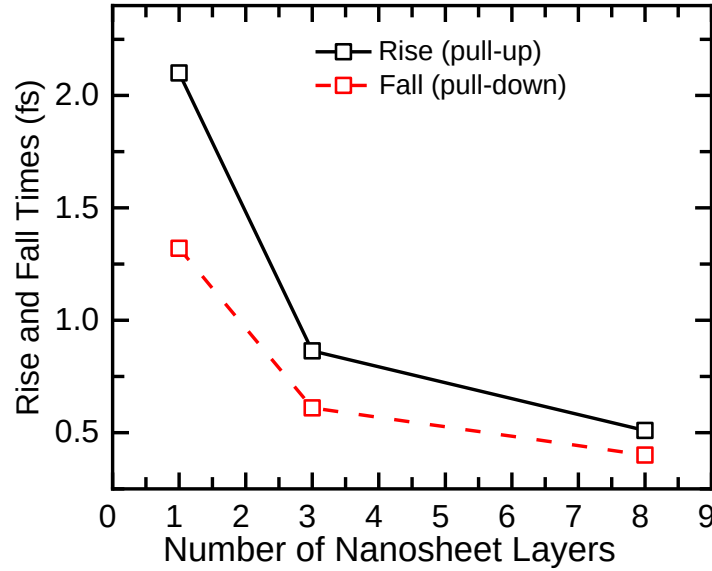


Figure 45. Improvement in rise and fall times with increasing number of nanosheet layers.

the p -NSFET and n -NSFET must have matched I_{ON} as well as threshold voltage (V_{TH}). Matching the threshold voltages ensures that the switching between the ON and OFF states occurs at nearly half the supply voltage (*here*, $V_{DD} = 0.5$ V) so that the inverter maintains high noise margins. In addition, a high-matched I_{ON} allows the inverter to switch from the ON state to the OFF state and vice versa at similar times and with fast switching, *i.e.*, stronger pull-up and pull-down networks. **Figure 44(a)** shows the structure of the NSFET-based inverter and **Figure 44(b)** shows the drain current versus gate voltage characteristics of both the 3-layer p -NSFET and 3-layer n -NSFET used to make the CMOS inverter. It is evident from **Figure 44(b)** that the switching voltage is near 0.25 V (*i.e.*, $V_{DD}/2$), as shown by the intersection of the individual curves. In addition, the I_{ON} are closely matched, with the n -NSFET having $\sim 1.29 \times$ more ON current than the p -NSFET due to the intrinsic difference in effective mobilities of electrons and holes.

Equal rising and falling transitions are essential for a symmetric response in CMOS circuits and are a cumulative function of the parasitic capacitances, parasitic resistances, load, geometry, and drive strength. Rise and fall times, measured from 10% to 90% time, are important parameters that determine the propagation delay as well as the frequency of operation. At low loads (*i.e.*, low fan-out), it is quite beneficial to use a transistor with low N to attain larger operating frequencies. As the load increased beyond a limit, a crossover was observed. On the other hand, at large loads, it is significantly beneficial to use a transistor with a higher number of nanosheets. **Figure 45** shows the impact of increasing the number of nanosheets on the rise and fall times of the inverter.

As the number of NS layers increases, the transition time decreases with higher I_{ON} . Therefore, it is critical to appropriately select the number of nanosheets used in the inverter design, based on the demands of the load, to attain the highest switching speeds possible.

In addition to a CMOS inverter, a 6-T SRAM circuit is simulated, as shown in **Figure 46**. The 6-T configuration was selected, as opposed to the 8-T or 10-T configurations, since it strikes a good balance between speed, power dissipation, and area occupancy [37]. SRAM circuits have three different functions: hold/standby, read, and write. Several SRAM metrics were evaluated such as read/write delay and noise margin. Static noise margins are important since they measure the stability of SRAM circuits, as shown in **Figure 46(a)** using butterfly curves. **Figure 46(b)** shows the static noise margins in all three modes. Read static noise margin (RSNM) is important since it measures the vulnerability of the circuit to bit errors during the read operation. Similarly, write static noise margin (WSNM) and hold static noise margin (HSNM) were evaluated as shown in **Figure 46(b)**. These metrics are almost independent of the number of nanosheets.

Furthermore, read and write delays are important metrics for determining the speed. The 50 fF capacitors were added to the bit lines to simulate a more realistic load environment for the SRAM circuits. As shown in **Figure 46(c)**, the read delay decreased by $\sim 30\%$ from 1 to 3 NS layers and by $\sim 10\%$ from 3 to 8 layers. On the contrary, the write delay increases linearly with additional NS layers due to the increased capacitive load present with more NS layers. Therefore, it is important to select the number of nanosheets appropriately for the read-and-write delay requirements.

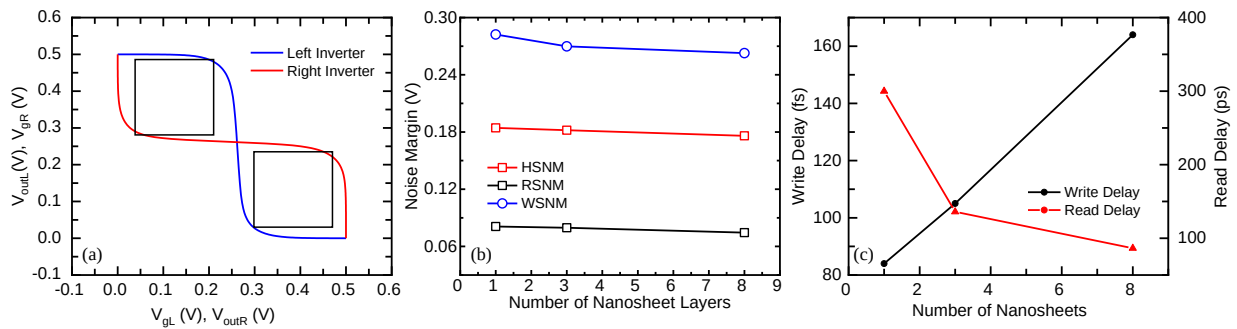


Figure 46. (a) Butterfly curves for Ge-on-AlAs NSFET-based 6-T SRAM configurations under read and write operations. Black square: graphical definition of read static noise margin (RSNM) and write static noise margin (WSNM). (b) Hold static noise margin (HSNM), RSNM, and WSNM as a function of number of nanosheet layers, and (c) both write and read delays as a function of number of nanosheet layers.

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Chapter 5 – Tensile Ge Quantum Well on-chip laser

5.1 The Physics of optical transitions in semiconductors

A typical chip-integrable semiconductor laser has three key components: an active region gain medium, a cavity for oscillations, and a p-n diode structure for current injection. The design of all three is crucial for optimum functionality. In most of the history of lasers, LEDs, and diode lasers, the gain medium has never been a non-emitting material. By this I mean, a material that fundamentally *does not* support the generation of light, *i.e.*, an indirect bandgap material. The gain medium is usually made using a III-V direct bandgap semiconductor [1-3]. Detailed reports of optical gain, gain enhancement, temperature dependence, and electrical threshold have been reported, leading to increasing performance and efficiency over the years [1-5] giving rise to the technological revolution discussed in **Chapter 1**. Thus, out of the three key components discussed above, the ability of the gain medium to produce light emission and consequently gain needs to be revisited along with methods to improve light generation. Ge-based light sources have a wide range of potential applications, but the material needs to be coerced to produce light first before proceeding with the design of other key components such as waveguide, cavity, structure, mode selection filtering, and contacts. Hence, this section revisits the fundamentals for light generation from semiconductors and the principles of lasing in the context of achieving lasing from an indirect bandgap material such as Ge.

The gain medium, for the intended wavelength of application, is usually an absorbing semiconductor layer. Incident photons of the right energy/frequency will easily excite electrons from the valance band to the conduction band. The condition for absorption of a photon of energy E_{ph} is that $E_{ph} > E_g$, which implies that the energy of the incident photon must be larger than the bandgap of the material. Interestingly, if the material is pumped or flooded with electrons through an external current source pushing the material into a non-equilibrium state, light emission is possible *i.e.*, the inverse of the absorption process. Such a device is called an electrically pumped laser and is the primary focus of this work. Optical pumping of the laser cavity is also possible and has been the focus of many studies [6].

The operation of semiconductor lasers is drastically different compared to typical gas lasers and an understanding of the band structure of solid-state materials encompassing Zinc-blende lattice semiconductors is required. Semiconductors are solids whose atoms form energy bands due

to proximity-induced splitting, each of which are solutions of the Schrodinger Equation for the individual atomic orbitals. The splitting is caused by the presence of two stable bonding configurations for the valence electrons of the two interacting atoms. These stable configurations are *bonding* and *anti-bonding*. The bonding configuration is symmetric, low energy, and has charge concentration present between the two atomic nuclei. The anti-bonding configuration is antisymmetric, high energy and the charge distribution lacks charges in between the two atomic nuclei. Hence, isolated energy levels of the individual atoms have now split into two energy levels. When a third atom is introduced in this picture, it creates a third level which is strictly speaking neither bonding nor anti-bonding. Similarly, when N such atoms in a crystalline solid come into proximity, complicated band splitting takes place forming the characteristic energy band structure of the material. This splitting and band formation is a consequence of covalent bonding between atoms in a solid crystal. Further, one must account for the electron spin degeneracy at each level allowing 2 electrons per eigenenergy, resulting in $2N$ levels, not N . The number N in a semiconductor solid is usually attributed to the number of unit cells, not individual atoms. The unit cell or the primitive cell typically has two atoms, resulting in one of them filling the upper energy level and the other one filling the lower energy level. The valence band is formed by the splitting of the highest occupied energy levels in the solid. Hence, the valence band is the highest energy level at 0 K which is completely occupied without the need for external energy through temperature, voltage, or light. Similarly, the conduction band is formed by the splitting of higher energy levels which are empty and require excitation in order to be populated. Excitation of the electrons from the valence band will result in their displacement into the conduction band, but while leaving a “hole” in the VB. This hole is a quasi-particle that will participate in the transport and carrier dynamics of the semiconductor material just like the electron. Each excited electron into the CB creates an electron carrier for conduction in the CB, while also creating a hole carrier in the VB.

The band structure at the center of the Brillouin zone has a minima associated with the CB and a maxima associated with the VB. The simplified version of this band structure or E-k diagram is shown in **Figure 47**. Such a representation is a good assumption for most Zinc-Blende crystals such as Si, Ge, and GaAs. For Si and Ge which are indirect bandgap materials, another band appears in the CB which is lower in energy than the one shown above, and a detailed discussion

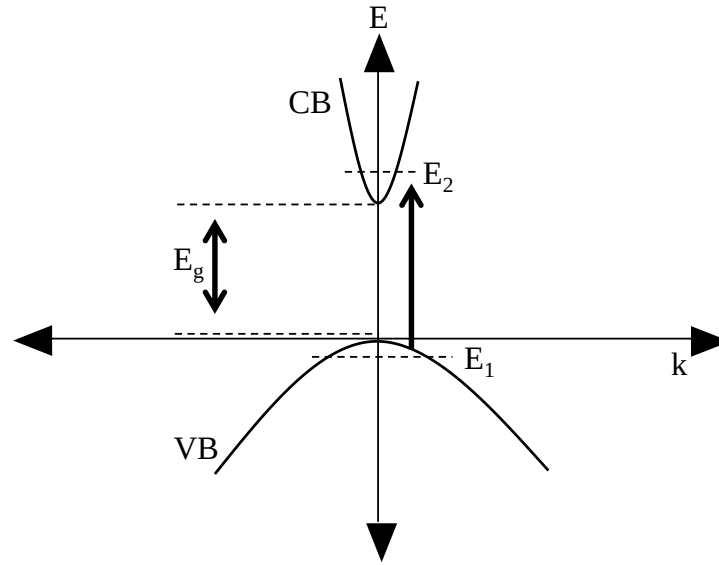


Figure 47. A simplistic version of a semiconductor crystal band structure with a CB and VB.

will be provided in this Chapter. For a transition to occur between two energy levels in the band structure, for example, an excitation of an electron in the VB at energy E_1 to an energy level E_2 in the CB as shown in **Figure 47** the energy difference between the two levels must be equal to or larger than the bandgap E_g . Thus, transitions of energy less than this are forbidden indicating that a photon of energy less than E_g cannot excite the electron from VB to CB.

Four general types of transitions are possible for a semiconductor. *Spontaneous recombination* results in photon emission due to an electron at energy E_2 relaxing and recombining with a hole at energy E_1 . This causes emission of a photon of energy equal to the difference $E_{ph} = E_2 - E_1$. Consider the case where a large number of these recombinations occur, the emission direction and time would be random resulting in an in-coherent radiation and these photons will not contribute to a coherent EM field. This is the principle of operation of typical LEDs used in commercial and scientific applications today. The recombination rate will be proportional to the available density of electron hole pairs $N \times P$, or roughly N^2 for undoped active regions. The second type is *stimulated generation or absorption* of a photon, the inverse of the process discussed above. A photon of energy $E_{ph} = E_2 - E_1$, or larger is absorbed by the electron at energy E_1 resulting in its excitation to the CB at energy E_2 . The third type is *stimulated recombination* which results in coherent photon emission. An incident photon of the appropriate energy $E_{ph} = E_2 - E_1$ is present in the cavity due to a pre-existing photon EM field. This photon stimulates the emission of another

photon of the same energy resulting in an addition in the pre-existing photon field. One can note the positive feedback present in this mechanism, and this is exactly what is required in a laser operation and what lacks in a LED, a positive feedback reflective cavity for the EM field. Lastly, a fourth mechanism exists which interferes with efficient gain generation in LEDs and Lasers. This is the non-radiative mechanism which causes relaxation of an electron in the CB through pathways other than the direct pathway shown in **Figure 47**. These non-radiative pathways include the participation of defects, interface traps, phonon exchanges. They result in heat dissipation and loss of carriers as well as gain, resulting in a higher current consumption, device heating as well as poor efficiency. A detailed discussion on non-radiative mechanisms, minority carrier lifetime and their impact is provided later in this Chapter.

A quantum mechanical description of photon emission through the recombination of electrons and holes requires a Hamiltonian associated with the interaction of the electron and photon, described as [1, 2],

$$H = \frac{1}{2m_0} (p - eA)^2 + V(r) \quad (5.1.1)$$

where m_0 is the mass of the free electron, A is the vector potential for the electromagnetic field, p is the momentum, and $V(r)$ is the periodic crystal potential associated with the semiconductor crystal. The quadratic term can be expanded to obtain,

$$H = \frac{p^2}{2m_0} + V(r) - \frac{e}{2m_0} (p \cdot A + A \cdot p) + \frac{A^2 e^2}{2m_0} \quad (5.1.2)$$

where the first two terms are the unperturbed Hamiltonian H_0 . The last term is quadratic in A and hence can be ignored as its much smaller than the linear terms. Using the Coulomb gauge, $\nabla \cdot A = 0$, resulting in $(p \cdot A = A \cdot p)$. This can be further simplified to,

$$H = H_0 + H' \quad (5.1.3)$$

where the first term is the unperturbed Hamiltonian H_0 , and the second term in the perturbation due to the interaction with the light. The vector potential A of the EM light wave is a sinusoidal wave of the form,

$$A = A_0 \cos(k \cdot r - \omega t) \vec{e} \quad (5.1.4)$$

where $\vec{e}$ is the unit vector in the direction of the electric field. The perturbation Hamiltonian can be written as,

$$H' = -\frac{e A_0 e^{ik \cdot r}}{2m_0} \vec{e} \cdot \mathbf{p} \quad (5.1.5).$$

This interaction Hamiltonian now describes the transition probability between two states in the band structure of a crystal semiconductor, similar to the two energy levels shown in **Figure 47**. For two states, a ground state and an excited state with eigen energies E_1 and E_2 , and wavefunctions $|a\rangle$ and $|b\rangle$ respectively, using **Fermi's Golden rule** derived from time dependent perturbation theory, the transition rate from $|a\rangle$ to $|b\rangle$ for such a 2-state system can be written as [1, 2],

$$W_{abs} = \frac{2\pi}{\hbar} |\langle b | H'(r) | a \rangle|^2 \delta(E_2 - E_1 - \hbar\omega) \quad (5.1.6).$$

This rate represents the transition rate for the process of absorption, when the incident photon of energy $E_{ph} = \hbar\omega$ is able to excite an electron from the eigen state $|a\rangle$ with ground state energy E_1 to an excited state with eigen energy E_2 and eigen state $|b\rangle$. The transition rate for absorption per unit volume for the crystal can be calculated for the case when the state $|a\rangle$ is occupied but $|b\rangle$ is not by summing over the initial and final states,

$$R_{abs} = \frac{2}{V} \sum_{k_a} \sum_{k_b} \frac{2\pi}{\hbar} |H'_{ba}|^2 \delta(E_2 - E_1 - \hbar\omega) \cdot f_a \cdot (1 - f_b) \quad (5.1.7).$$

Where the Fermi-Dirac distribution calculated fractions f_a and $(1 - f_b)$ represent the probabilities of the state $|a\rangle$ being occupied and the state $|b\rangle$ being empty respectively. The additional factor 2 which is present above is due to the spin degeneracy. The matrix element notation is introduced for the transition here, $|H'_{ba}|^2$ which is obtained from Eq 5.1.6 expanding the bra-ket product,

$$H'_{ba} = \langle b | H'(r) | a \rangle = \int \psi_b^* \cdot H'(r) \cdot \psi_a dV \quad (5.1.8).$$

A few intuitive changes can modify this equation, preserving the physical nature and describing the inverse process for light emission. Light emission requires that the state $|b\rangle$ be occupied and the state $|a\rangle$ be empty and the transition rate with the perturbation Hamiltonian conjugate ($H'(r)^*$) for the emission process (generation of a photon) can be written as,

$$W_{emit} = \frac{2\pi}{\hbar} |\langle a | H'(r)^* | b \rangle|^2 \delta(E_1 - E_2 + \hbar\omega) \quad (5.1.9).$$

Finally, the total emission rate can be calculated as,

$$R_{emit} = \frac{2}{V} \sum_{k_a} \sum_{k_b} \frac{2\pi}{\hbar} |H'_{ab}|^2 \delta(E_1 - E_2 + \hbar\omega) \cdot (1 - f_a) \cdot f_b \quad (5.1.10).$$

In a semiconductor, the absorption and emission processes described above take place simultaneously in a competing manner. In equilibrium, they are equal and there is no net absorption or emission of photons. The net emission rate (for a fixed photon energy $\hbar\omega$) can be defined as the difference between the two competing rates described above,

$$R_{net} = R_{emit} - R_{abs} = \frac{2}{V} \sum_{k_a} \sum_{k_b} \frac{2\pi}{\hbar} |H'_{ba}|^2 \delta(E_2 - E_1 - \hbar\omega) \cdot (f_b - f_a) \quad (5.1.11).$$

This is the net emission rate per unit volume for a monochromatic electromagnetic field in the lasing cavity, central to the gain calculations discussed in later sections. Note that as the electromagnetic field is monochromatic, the term $\hbar\omega$ is fixed. If we wish to calculate the transition

rates in a cavity with a broad distribution of the electromagnetic field, the photon number distribution in accordance with the Bose-Einstein statistics needs to be considered.

For a broad-spectrum EM field in the cavity, the photon number follows the Bose-Einstein statistics with energy $\hbar\omega_k$ for the frequencies ω_k according to,

$$n_p = \frac{1}{e^{\hbar\omega_k/k_B T} - 1} \quad \text{with } \omega_k = \frac{k \cdot c}{n_r} \quad (5.1.12).$$

In k-space, the unit volume is $V = (2\pi/L)^3$ and the number of states in a differential volume in k-space is

$$N(E_{21}) = \frac{2}{V} \sum \delta(E_2 - E_1 - E_k) \quad (5.1.13).$$

It can be shown that for an energy gap of E_{21} between the two energy levels the number of states per unit volume per unit energy interval is,

$$N(E_{21}) = \frac{n_r^3}{\pi^2} \frac{E_{21}^2}{\hbar^3 c^3} \quad (5.1.14).$$

An interesting relation is found, relating the number of photon states or “photonic density of states” to the refractive index n_r and the energy gap E_{21} . Now that the photon states in the cavity per unit energy gap is quantified, we can proceed to calculate the transition rates for stimulated and spontaneous emission. The upward (absorptive) transition rate per unit volume by taking the product of, (i) transition rate per incident photon $B_{12} = \frac{2\pi}{\hbar} |H'_{12}|^2$, (ii) number of photon states per unit energy per unit volume $N(E_{21})$, and (iii) the average number of photons n_p per state according to the Bose-Einstein statistics in the energy gap E_{21} . Notice that the units/physical dimensions should line up, B_{12} has units of eV/s , $N(E_{21})$ has units of $(cm^{-3} eV^{-1})$ and the number n_p is unitless. Hence the total product of the three has units of $(cm^{-3} s^{-1})$, *i.e.*, transition rate per unit volume, as expected [1, 2]. This product is the absorptive transition rate while exciting an electron from $1 \rightarrow 2$, per unit volume for a broad spectrum radiation, denoted by R_{12} .

As the carriers follow the Fermi-Dirac statistics, considering the probabilities of occupation of these states, *i.e.*, state 1 being filled is f_1 and state 2 being empty is $(1 - f_2)$, the expression for the transition rate per unit volume can be written as,

$$R_{12} = \frac{1}{V} \sum B_{12} \delta(E_2 - E_1 - E_k) \cdot 2n_p \cdot f_1 \cdot (1 - f_2) \quad (5.1.15),$$

further simplified as,

$$R_{12} = B_{12} N(E_{21}) \cdot n_p \cdot f_1 \cdot (1 - f_2) \quad (5.1.16).$$

The transition rate R_{12} (Eq 5.1.16) is the transition rate per unit volume for the ***stimulated absorption process*** where an incident photon excites an electron from the VB to the CB. Consequently, the ***stimulated emission process*** where the incident photon induces the relaxation of an electron in the CB to recombine with a hole in the VB can be defined as,

$$R_{st} = B_{21} N(E_{21}) \cdot n_p \cdot f_2 \cdot (1 - f_1) \quad (5.1.17).$$

Noting a few critical changes, the transition rate B_{21} is now between $2 \rightarrow 1$ and the fermi factors represent the probability of state 2 being filled, f_2 and the probability of the state 1 being empty $(1 - f_1)$. A third important process, ***spontaneous emission*** exists due to an interaction with the vacuum field. This can be thought of as a stimulated emission due to the vacuum fluctuations generated photons. Hence, it is independent of the photon number in the cavity, resulting in a transition rate for ***spontaneous emission*** given by,

$$R_{spon} = A_{21} f_2 \cdot (1 - f_1) \quad (5.1.18).$$

When the material is in thermal equilibrium, there will be a single fermi level and the total upward transitions will be equal to the total downward transitions.

$$\text{In Equilibrium:} \quad R_{12} = R_{spon} + R_{st} \quad (5.1.19).$$

Using Eq 5.1.19 and Eq 5.1.14, the rate constant A_{21} can be determined to be,

$$A_{21} = N(E_{21}) \cdot B_{21} = \frac{n_r^3}{\pi^2} \frac{E_{21}^2}{\hbar^3 c^3} \cdot B_{21} \quad (5.1.20).$$

Similarly, the ratio of the stimulated emission rate to the spontaneous emission rate is simply the number of photons per state,

$$\frac{R_{st}}{R_{spon}} = n_p \quad (5.1.21).$$

The net absorption rate will be the difference of the two competing mechanisms, stimulated absorption and stimulated emission,

$$R_{abs} = R_{12} - R_{st} = B_{12} \cdot (f_1 - f_2) \cdot N(E_{21}) \cdot n_p \quad (5.1.22).$$

Summing over all the initial states and final states, the absorption spectrum for a given spectral energy $E_k = \hbar\omega_k$ is given by,

$$\alpha(\hbar\omega) = \frac{2 n_r}{c} \sum_{k_1} \sum_{k_2} B_{12} \delta(E_2 - E_1 - \hbar\omega) (f_1 - f_2) \quad (5.1.23).$$

Noting that finite non-zero absorption will only take place when the $\delta(E_2 - E_1 - \hbar\omega)$ function has a value of 1, which is possible only when the energy difference in the two states $E_2 - E_1$ is equal to the energy of the interacting photon $\hbar\omega$. This is a consequence of energy conservation indicating that the transition is only possible when the two states are separated by $\hbar\omega$. Using the time averaged power density in the EM wave associated with the perturbation Hamiltonian, we can define the Poynting vector P , *i.e.*, the photon's optical intensity for volume V in a medium with refractive index n_r , the interaction Hamiltonian discussed in Eq 5.1.5 and Eq 5.1.8 can be simplified as [1, 2],

$$B_{12} = \frac{\pi e^2}{n_r^2 \epsilon_0 m_0^2 \omega} \frac{1}{V} |\langle \vec{e} | p \rangle|^2 \quad (5.1.24).$$

The Poynting vector P equated to the optical intensity is,

$$P = \hbar \omega_k \frac{c}{V n_r} = \frac{n_r c \epsilon_0 \omega^2 A_0^2}{2} \quad (5.1.25).$$

Finally, the stimulated emission rate per unit energy interval can be derived as,

$$r_{st}(\hbar\omega) = \frac{2 n_r^2 \omega^2}{\pi^2 \hbar V c^2} C_0 \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \delta(E_2 - E_1 - \hbar\omega) (f_2 - f_1) \quad (5.1.26).$$

Where the constant $C_0 = \frac{\pi e^2}{n_r c \epsilon_0 m_0^2 \omega}$, and the gain spectrum and absorption spectrum are related as $g(\hbar\omega) = -\alpha(\hbar\omega)$ from Eq. 5.1.23. Hence, the gain $g(\hbar\omega)$ in the cavity can be defined in the context of *stimulated emission rate* as,

$$r_{st}(\hbar\omega) = \frac{n_r^2 \omega^2}{\pi^2 \hbar c^2} g(\hbar\omega) \quad (5.1.27)$$

from Eq. 5.1.26. Also, the *spontaneous emission rate* per unit energy interval can be determined from,

$$r_{spont}(\hbar\omega) = \frac{2 n_r^2 \omega^2}{\pi^2 \hbar V c^2} C_0 \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \delta(E_2 - E_1 - \hbar\omega) f_2 (1 - f_1) \quad (5.1.28)$$

with only a change in the fermi factors at the end. Note that the terms discussed here, $g(\hbar\omega)$ and $\alpha(\hbar\omega)$ are the gain spectrum and the absorption spectrum respectively, not to be confused with the gain/absorption coefficients which are slightly different as shown below,

$$Abs\ Coeff \rightarrow \alpha(\hbar\omega) = \frac{2}{V} C_0 \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \delta(E_2 - E_1 - \hbar\omega) (f_1 - f_2) \quad (5.1.29).$$

The delta function may be replaced with a broadening function depending on the type of transition, a common choice of broadening function is the Lorentzian Function.

5.2 Gain in a laser diode: Fermi levels, Transition strengths, and DOS

After reviewing the various transition rates, it is evident that the gain for the laser is proportional to the stimulated emission rate. This rate along with Fermi's Golden rule defines a “internal” quantum mechanical gain and absorption spectrum. But gain or light emission is only possible when external stimulation is applied, in this section we add on to the previous section by elaborating on the inclusion of fermi levels, applied voltage, wavefunctions, transition matrix and DOS for a bulk material. The Fermi factors (f_1 and f_2) used in the transition rate calculation in the

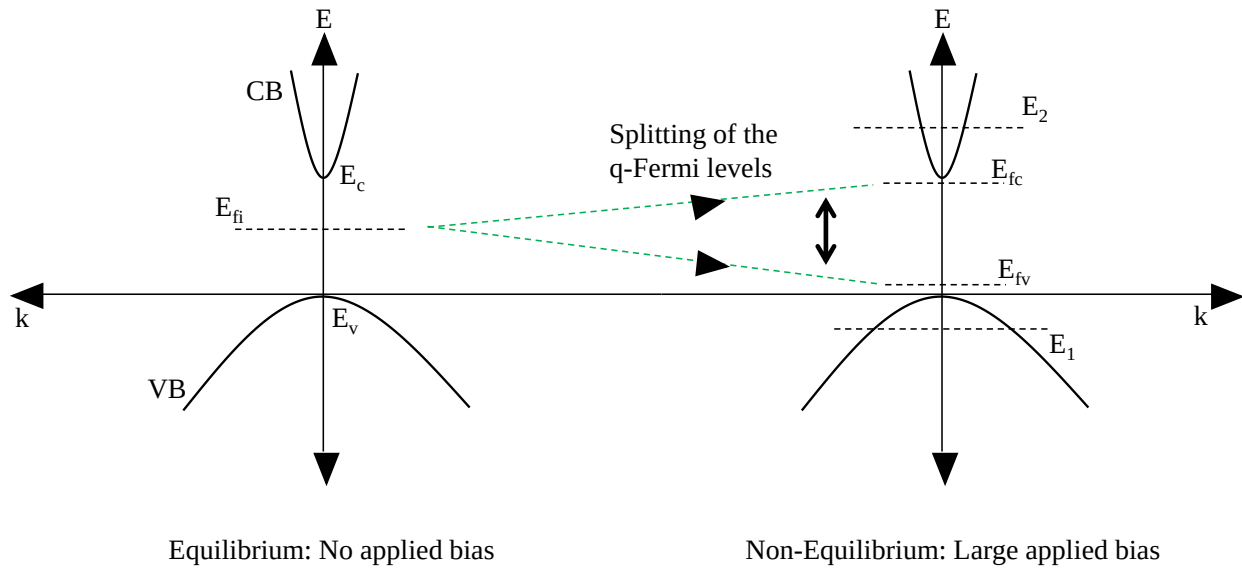


Figure 48. Splitting of the fermi level due to applied bias resulting in the formalization of electron and hole quasi-fermi levels.

previous section depend on the current injection in the semiconductor through the quasi-fermi level formation. When a given material is in equilibrium, only one intrinsic fermi level exists, however, upon application of a large voltage/current bias the fermi level splits into quasi-fermi levels for the electrons and holes as shown in **Figure 48**. The material has now moved to a non-equilibrium state due to the applied bias and contains a large number of electrons and holes. The exact densities of electrons and holes in this condition is determined by the temperature, applied bias, relative fermi level separation and intrinsic carrier concentration associated with the band gap of the material. The occupation probability for an electron at energy E_1 and E_2 shown here can be quantified using the Fermi-Dirac distribution as,

$$f_1 = \frac{1}{1 + e^{\left(\frac{E_1 - E_{fv}}{k_B T}\right)}} \quad \text{and} \quad f_2 = \frac{1}{1 + e^{\left(\frac{E_2 - E_{fc}}{k_B T}\right)}} \quad (5.2.1).$$

Here E_{fv} and E_{fc} are the hole and electron quasi-fermi levels respectively. Consequently, the stimulated absorption and stimulated emission rates can be compared based on Eq. 5.1.15 and Eq. 5.1.16 such that,

$$\frac{R_{st}}{R_{abs}} = \frac{f_2 (1 - f_1)}{f_1 (1 - f_2)} \quad (5.2.2).$$

The factor $(1 - f_1)$ indicates the absence of an electron at the energy E_1 , actually signifying an empty state or the presence of a hole. If the ratio in Eq. 5.2.2 is greater than 1, the stimulated emission is greater than the absorption and we have net gain. Using Eq. 5.2.2 and Eq 5.2.1, the ratio can be further simplified to,

$$\frac{R_{st}}{R_{abs}} = e^{\left(\frac{\Delta E_f - E_{21}}{k_B T}\right)} \quad (5.2.3).$$

Revealing an important condition for lasing, known as the Bernard and Durauffourg rule indicating that the net gain is possible when the ratio in Eq. 5.2.3 is greater than 1, or

$$\Delta E_f - E_{21} > 0 \rightarrow E_{fc} - E_{fv} > E_{21} \quad (5.2.4).$$

The fermi level separation created by the applied bias/voltage should be larger than the energy of the photon of interest, in order to produce net gain. In semiconductors, the minimum allowed separation for a transition is the energy band gap E_g . Photon energies lower than E_g are in most cases forbidden, thus modifying Eq. 5.2.4 to $E_{fc} - E_{fv} > E_g$. A fermi level separation larger than the bandgap of the material in the active region of the laser is required in order to produce net gain. The fermi level separation created is directly proportional to the applied external voltage across this p-n junction laser diode.

In the earlier section, through Eq. 5.1.5 to 5.1.9 the term $H'_{ba} = \langle b | H'(r) | a \rangle$ was introduced. It represents the magnitude of the matrix element of the overlap between the initial and final wavefunction while interacting with the interaction perturbation of the EM wave. We can now further simplify it here in the context of a semiconductor with a 2-band band structure. This matrix element determines the strength of the interaction or the transition between the two states. Certain transitions are allowed, some are forbidden. Two key terms in the expression are not yet known, the wavefunctions of electrons in the semiconductors at the initial and final states. The states $|a\rangle$ and $|b\rangle$ are wavefunctions obtained by solving the Schrodinger Equation. This can be simplified using the periodic nature of the atomic potential in the crystal as per the Bloch wave formulation ($u_v(r)$ and $u_c(r)$),

$$\psi_1 = F_1(r) \cdot u_v(r) \text{ and, } \psi_2 = F_2(r) \cdot u_c(r) \quad (5.2.5).$$

The functions $F_1(r)$ and $F_2(r)$ are envelope functions which represent the macroscopic potential created for the active region. This could be composition or doping difference created to change the band structure to create a potential profile. Usually, this potential profile in optoelectronic devices such as lasers, LEDs and detectors is a double heterostructure, quantum well, or a quantum dot. Using Eq. 5.2.5, the wavefunction has been split into two product terms, one associated with the periodic potential of the crystal lattice atoms and the other is a macroscopic potential for the heterostructure. Here, $u_v(r)$ is Bloch wave for the electrons in the VB and $u_c(r)$ is the Bloch wave for the electrons in the CB. For a bulk system where the macroscopic potential is nearly constant over a very large distance, the envelope function can be derived as,

$$\text{Bulk system : } F(r) = e^{(-j k \cdot r)} / \sqrt{V} \quad (5.2.5).$$

For a quantum well active region where the macroscopic potential has a discontinuity in the potentials forming a “well”, the envelope function can be described as,

$$\text{QW system : } F(r) = e^{(-j k \cdot r_{\parallel})} / \sqrt{A} \quad (5.2.6).$$

The position vector $r_{\parallel}$ is the vector parallel to the quantum well plane. We can now substitute the wavefunction from Eq. 5.2.5 and Eq. 5.1.5 into Eq. 5.1.8 for the matrix element, to get,

$$H'_{21} = \langle b | H'(r) | a \rangle = \frac{e}{2m_0} \langle u_c | \vec{e} \cdot p | u_v \rangle \int F_2^* A(r) F_1 d^3r \quad (5.2.7).$$

Assuming that the EM plane wave varies slowly over the heterostructure, $A(r)$ can be assumed to be constant for the integral thus moving out of the integral. Thus, the matrix element can be written as,

$$|H'_{21}|^2 = \left(\frac{e A(r)}{2m_0} \right)^2 |M_T|^2 \text{ where } |M_T|^2 = |\langle u_c | \vec{e} \cdot p | u_v \rangle|^2 |\langle F_1 | F_2 \rangle|^2 \quad (5.2.8).$$

The term $|M_T|^2$ is the transition matrix element. The first term in it, $|\langle u_c | \vec{e} \cdot p | u_v \rangle|^2$, contains an EM polarization dependence on the band structure symmetries for the VB and CB. For a given material and for a given polarization, this momentum matrix element is constant and found through tabulated data via experiments. **However, a key deviation from conventional laser studies arises at this point while considering tensile Ge lasers (Chapter 5), GeSn lasers (Chapter 7) and the corresponding momentum matrix element.** The tensile strain changes the band structure of Ge, this further results in a change in the emissions rates from the various bands. Further, the preferred/dominant polarization from the two VBs is different resulting in the inability to keep the transition matrix element or the momentum matrix element constant. The following sections discuss how this varying momentum matrix element for tensile strained Ge in a quantum well configuration is calculated and used in the gain calculation for the TE and TM polarized light.

Before proceeding to the gain calculation quantum wells, a ***k-selection rule*** for bulk active regions can be formalized from Eq. 5.2.8. This k-selection rule can also be interpreted as ***momentum conservation*** indicating that the electron wavefunctions for the initial and final states should be aligned. Evaluating the overlap of the envelope functions as the volume of the region tends to infinity,

$$|\langle F_1 | F_2 \rangle| = \frac{1}{V} \int F_2^* F_1 d^3r = \frac{1}{V} \int e^{(j k_2 \cdot r)} e^{(-j k_1 \cdot r)} d^3r = \delta_{k_1, k_2} \quad (5.2.9).$$

This will have a non-zero value only when the vectors match, i.e., $k_1 = k_2$. Only states propagating in the same direction can interact and participate in optical transitions.

Up till now in these discussions, the electron transitions were occurring from a single state to a number of different final states. But in semiconductors, a continuous distribution of initial and final states exists resulting in a density of states available for the joint transition. This reduced density of states $\rho_r(E_{21})$, and within a small range of k values δk the CB energy range will be $\delta E_2 = \frac{\rho_r}{\rho_c} \delta E_{21}$ and $\delta E_1 = \frac{\rho_r}{\rho_v} \delta E_{21}$. The reduced density of states can be defined as [1, 2],

$$\frac{1}{\rho_r} = \frac{1}{\rho_c} + \frac{1}{\rho_v} \quad (5.2.10).$$

An expression for ρ_r which highlight the k -dependence of the energy bands is of importance while evaluating the DOS and reduced DOS for materials with many different bands, as shown here,

$$\frac{1}{\rho_r(E_{21})} = \frac{1}{\rho(k)} \left(\frac{dE_2(k)}{dk} - \frac{dE_1(k)}{dk} \right) \quad (5.2.11).$$

This enables the evaluation of ρ_r at any given k point as long as the dispersions of the electron and hole band energies are known. The dispersions of electron and hole band energies are usually well known due to the parabolic assumption which works well for most zinc-blende semiconductors. This expression shown in Eq. 5.2.11 becomes most critical in the few situations when the band structure is not parabolic. Here, we have introduced the DOS as a function of energy and k , the expressions for them for a bulk 3D structure are,

$$\text{Bulk 3D structure: } \rho(k) = \frac{k^2}{\pi^2}, \quad \rho(E) = \frac{\sqrt{E}}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \quad (5.2.12).$$

For a reduced dimensionality structure such as a quantum well, the expressions become,

$$\text{Quantum Well 2D structure: } \rho(k) = \frac{k}{\pi t_{QW}}, \quad \rho(E) = \frac{m}{\pi \hbar^2 t_{QW}} \quad (5.2.13).$$

Here the term t_{QW} represents the quantum well thickness which is of the order of ~ 10 nm in most quantum well structures.

The gain can now be computed for a semiconductor under an applied bias based on the expression derived in Section 5.1 and 5.2 through Eq. 5.1.6, 5.1.11, 5.1.13, 5.1.14, 5.1.17, 5.1.24, 5.1.25 as well as Eq 5.2.1 and 5.2.8.

$$g(E_{21}) = \frac{\pi e^2 \hbar}{n_r \epsilon_0 c m_0^2} \frac{1}{E_{21}} |M_T|^2 \rho_r(E_{21}) (f_2 - f_1) \quad (5.2.14)$$

5.3 A Tensile Strained Ge Quantum well laser: Physics and Computation

Now that the general expression for gain is defined for a semiconductor with two bands as shown in Eq. 5.2.14, a modification of the expression for a QW configuration for the active region is introduced. Further, the formation of a Ge QW creates unique consideration for sub-bands for the 2 VBs and 1 CB. The expression for gain needs to sum over the bands and their corresponding

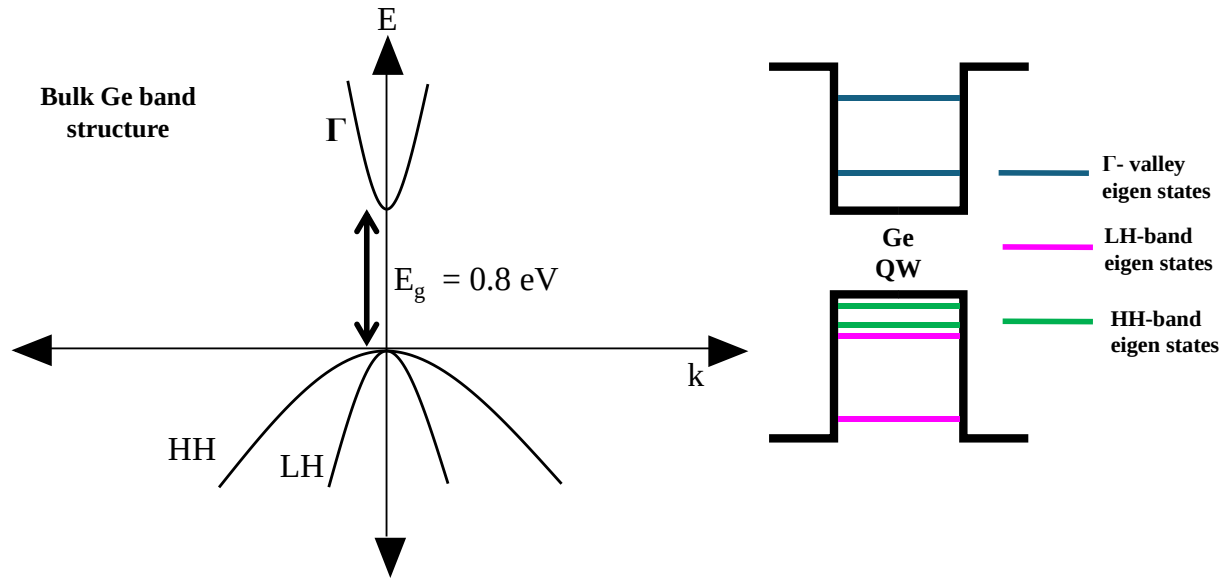


Figure 49. The band structure for bulk Ge showing the presence of 2 VBs and 1 CB at the Γ -point. (right) A Ge quantum well formed using barriers on both sides creating a well-potential profile. The first two eigen energies for each of the bands is shown.

sub-bands. The various bands in bulk Ge as well as the sub-bands formed after quantum well formation is shown in **Figure 49**. Like most zinc-blende lattice semiconductors, heavy hole and light hole VBs are present. The direct bandgap of Ge at room temperature is around 0.8 eV. Another VB associated with the spin-orbit coupling is present roughly 0.3 eV below the HH and LH bands, and will be discussed in **Chapter 7**. After the formation of a quantum well where Ge is sandwiched in between two high band gap materials such as InGaAs or InAlAs, the energy levels are quantized provided the thickness of the Ge layer is small roughly of the order of 10 nm. The 3 dominant bands shown here will have quantized energy levels and sub-bands will form corresponding to each of them, Γ , LH and HH. Considering radiative transitions between the CB and the VB, each CB sub-band electron can recombine with a hole in either the HH band or the LH band, each having multiple sub-bands. This creates a multitude of transition possibilities, and

for accurate gain calculation we will sum over all of these combinations. Fortunately, some of these transitions are deemed unlikely or have nearly no probability of occurring. So, in the following discussion, some of these transitions are eliminated using the k-selection rule.

Similar to the k-selection rule discussed in Eq. 5.2.9 for bulk structures, we can evaluate the overlap integral for the Ge quantum well shown in **Figure 49**,

$$|\langle F_1 | F_2 \rangle| = \frac{1}{A} \int F_2^*(z) e^{(j k_2 \cdot r_{\parallel})} F_1(z) e^{(-j k_1 \cdot r_{\parallel})} d^3 r \quad (5.3.1).$$

Applying similar k-selection, $k_1 = k_2$ the integral can reduce to,

$$|\langle F_1 | F_2 \rangle| = \frac{1}{A} \int F_2^*(z) F_1(z) d^3 r \quad (5.3.2).$$

Noting that the quantum well wavefunctions are orthogonal and the integral can be further reduced to,

$$|\langle F_1 | F_2 \rangle| = \delta(n_1, n_2) \quad (5.3.3).$$

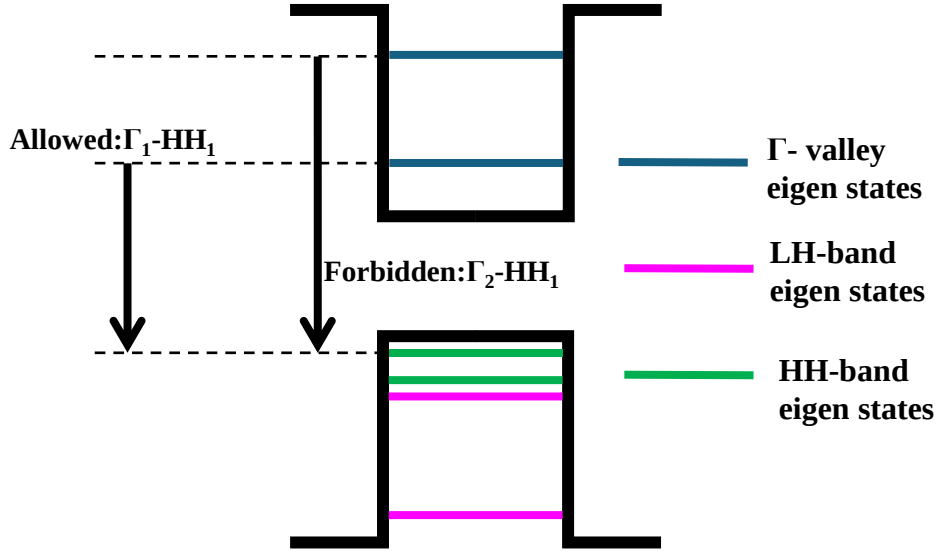


Figure 50. An example of an allowed and forbidden transition in a Ge QW.

Where n_1 and n_2 are quantum numbers of the sub-bands in the QW. This implies that only the transitions between sub-bands which have the same quantum number n are possible. Thus, transitions between the first sub-band in the Γ valley are possible with the first sub-band in the LH and HH band, but not with the second or third. This reduces the number of sub-bands which can participate in allowed transitions as well as the number of bands we need to integrate over for the gain calculation of the quantum well. Transition between sub-bands which don't follow the k-selection rule have different quantum numbers and are forbidden, but in the presence of defects, large dopant concentrations and finite offsets, they can have a minute presence. An example of an allowed transition between the first sub-band ($n = 1$) in the Γ valley and the first sub-band ($n = 1$) in the HH-band is shown below in **Figure 50**. Similarly, a transition which doesn't follow the discussed k-selection rule is shown between the second sub-band ($n = 2$) in the Γ valley and the first sub-band ($n = 1$) in the HH-band, such a transition is forbidden [1, 2].

The total material gain can be extended from Eq. 5.2.14 to include all the allowed sub-bands in the Ge QW as well as a Lorentzian broadening function ($L(E_2 - E_1 - \hbar\omega)$ i.e., the last factor in Eq 5.3.4 below) with an intra-band relaxation time of $\tau_{in} = 0.1$ ps,

$$G(E_{21}) = \int \sum_{LH,HH} \sum_{n_q} \frac{\pi e^2 \hbar}{n_r \epsilon_0 c m_0^2} \frac{1}{E_{21}} |M_T|^2 \rho_r(E_{21}) (f_2 - f_1) \frac{\left(\frac{\hbar}{2\pi\tau_{in}}\right)^2}{\left(\frac{\hbar}{2\pi\tau_{in}}\right)^2 + (E_{21} - E)^2} \cdot dE \quad (5.3.4)$$

Also, here we move to represent the gain with *upper-case* G instead of *lower-case* g, as later g will represent the modal gain whereas G is the material gain in Eq. 5.3.4. Most of these terms are material parameters of Ge and physical constants, so the material gain can be calculated directly. Interestingly, applying a small biaxial epitaxial tensile strain changes the band structure of Ge resulting in the formation of two important direct bandgaps, Γ -HH and Γ -LH and their corresponding sub-bands. Further, the polarization dependence of LH and HH wavefunctions is distinct thus affecting $|M_T|^2$ which will no longer be constant. These band edges, Γ -HH and Γ -LH move distinctly with tensile strain, resulting in a tensile strain dependence for the transition energy, polarization, JDOS and to a certain extent, refractive index.

Depending on the magnitude of the band-offset in the potential well seen in **Figure 50**, the number of eigen energies confined in the well can be estimated. As an approximation, considering that the well is infinitely deep, the eigen energies are given by,

$$\text{Eigen energies of a QW: } E_n = \frac{\pi^2 \hbar^2}{2 m^* t_{QW}^2} n^2 \quad (5.3.5).$$

Here, the number n is the quantum number associated with the sub-band, m^* is the effective mass of the carrier in the particular band, and t_{QW} is the quantum well thickness. The first energy, i.e., the ground state is not at the energy 0, but at a finite number usually of the order of 50 meV. It has a dependence as shown in Eq. 5.3.5. Noting the dependence of the consecutive higher sub-bands on n^2 , the next sub-band will be of the order of ~ 200 meV and the third would be 450meV. The band offsets need to be larger than this energy value for the electron to remain bound. For example, if the electron has an energy of 300 meV, but the band offset in the quantum well is only 200 meV, the electron will not be bound in the quantum well. The exact values of the band offset in this tensile Ge and InGaAs QW system will be discussed later. But for all intents and purposes, this finite-offset quantum well holds 1-2 eigen energy levels for the Γ -valley as the band offset for the CB is between 200 - 400 meV. Considering just these two important sub-bands ($n = 1, 2$) for the

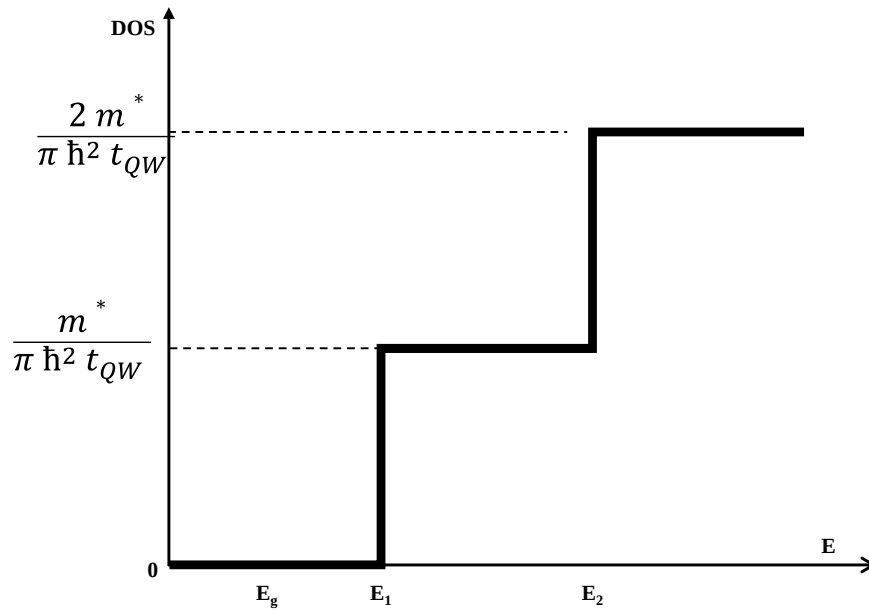


Figure 51. The Density of states as a function of band energy in the Ge QW

CB Γ -valley enables us to also ignore $n > 2$ sub-bands in the VB for the LH and HH bands. This is due to the k-selection rule discussed earlier. So, in Eq. 5.2.4, the summation needs to cover two values of the quantum number $n_q = 1, 2$, and two values of the transition bands either LH or HH. This narrows down the summation in Eq. 5.2.4 to 4 terms, one for each of the transition peaks: ground state transitions (A: $E_{pk(\Gamma1-LH1)}$, B: $E_{pk(\Gamma1-HH1)}$) and the first excited state transitions (C: $E_{pk(\Gamma2-LH2)}$, D: $E_{pk(\Gamma2-HH2)}$). The DOS for each of the sub-bands to be used in Eq. 5.2.4, is a staircase

Heaviside function with the magnitude dependent on the effective mass of the band as shown in **Figure 51**. Such a distribution will exist for the VB LH and VB HH as well, and a reduced DOS $\rho_r(E_{21})$ will be computed for the two bands participating in the transition.

Another important term that will be affected significantly as the tensile strain in the Ge QW moves the bands, is the polarization-dependent transition matrix element $|M_T|^2$, which is proportional to the momentum matrix element $|M|^2$ and the overlap of the envelope functions used in Eq. 5.3.3. The polarization (TE vs TM) dependence of transitions can be understood using the relative transition strength associated with the two interacting eigenstates and their corresponding wavefunctions. This relative transition strength is defined as the ratio of the transition matrix element and the momentum matrix element $\frac{|M_T|^2}{|M_0|^2}$. Consequently, this ratio will determine the relative transition probability of various transitions between sub-bands under consideration [1, 2]. In the ε -Ge/InGaAs QW laser structure, the degeneracy between LH and HH bands is broken due to the biaxial tensile strain, and transitions from their corresponding sub-bands would be competing for gain while also resulting in different polarizations (TE or TM) of light. Also, the cavity will support many other modes, and the accurate optical polarization would be quasi-TE or quasi-TM, here the analysis is done for the fundamental mode only. In the case of a bulk Ge as the lasing medium, the Γ -LH and Γ -HH relative transition strength would be equal for the TE and TM modes. But in QW structures, this relative transition probability is re-distributed between TE and TM modes unequally, the Γ -LH transition would only contribute to the material gain of the TM mode (G_{TM}) and the Γ -HH transition would contribute largely to the material gain of the TE mode (G_{TE}). The calculation of these transition matrix elements (between n^{th} sub-bands following k-selection) proceeds through the calculation of the overlap integrals between the interacting wavefunctions QW given by [1, 2],

$$|M_T|^2 = |M_0|^2 \left\{ \frac{2}{3} |\langle \psi_{\Gamma,n} | \psi_{LH,n} \rangle|^2 \right\}, \quad \text{for the TM mode} \quad (5.3.6),$$

$$|M_T|^2 = |M_0|^2 \left\{ \frac{1}{6} |\langle \psi_{\Gamma,n} | \psi_{LH,n} \rangle|^2 + \frac{1}{2} |\langle \psi_{\Gamma,n} | \psi_{HH,n} \rangle|^2 \right\}, \quad \text{for the TE mode} \quad (5.3.7).$$

where, $\psi_{\Gamma,n}$ is the normalized wavefunction of the n^{th} sub-band electron in the Γ -valley, $\psi_{\text{LH},n}$ and $\psi_{\text{HH},n}$ are the normalized wavefunctions of the n^{th} sub-band holes in the LH and HH band, respectively. Thus, with the application of tensile strain distinct considerations of gain and optical confinement for the various transitions and corresponding TE and TM polarization of the output are required to determine which transitions ultimately lase. The momentum matrix element $|M_0|^2$ is determined through the modified expression for each transition [1, 2],

$$|M_0|^2 = (m_0 E_g / 2) \left(\frac{m_0}{m_{\text{eff},e}} - 1 \right) \left(\frac{E_{tr,n} + so}{E_{tr,n} + \left(\frac{2}{3}\right) so} \right) \quad (5.3.8).$$

where, $m_{\text{eff},e}$ is the effective mass of the electron in the conduction band and so is the energy of the spin-orbit VB energy assumed to be 0.29 eV for Ge. The term $E_{tr,n}$ is the transition energy associated with the transition between the two sub-bands and is a function of tensile strain as well as the eigen energies of the bands. The term E_g is simply the bulk bandgap of Ge, roughly ~ 0.8

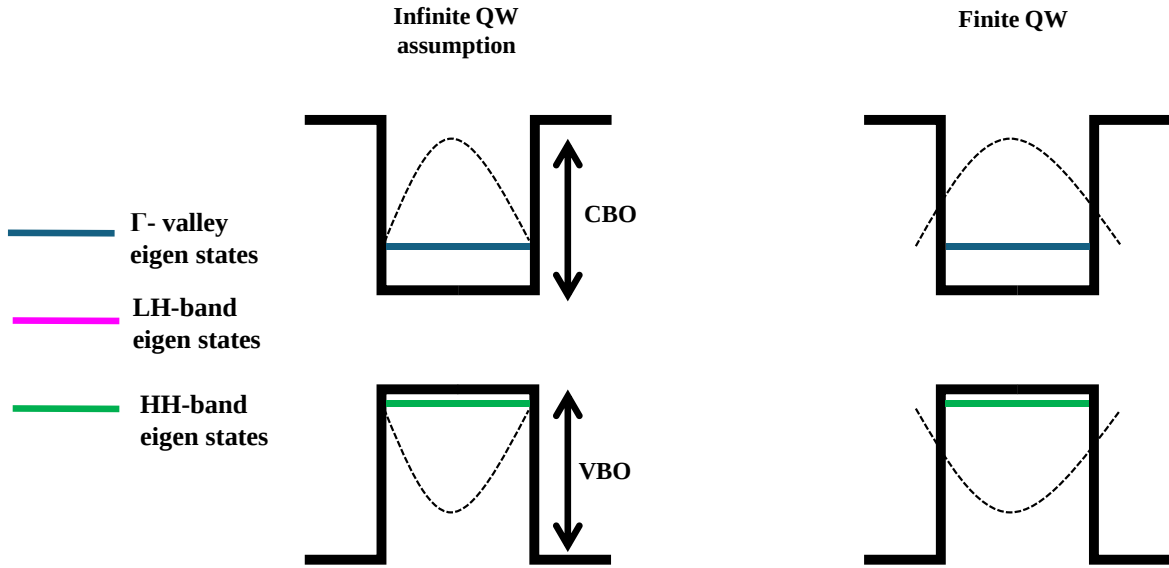


Figure 52. Wavefunctions in an infinite and finite QW. The finite QW is a realistic description where the wavefunction leaks into the barrier.

eV and is also drastically dependent on the applied tensile strain. In essence, it is evident that for gain calculations of a tensile strained Ge laser, the momentum matrix element which is usually a material constant for most lasing studies, cannot be assumed to be constant.

Finally, an important distinction needs to be made in order to complete the discussion of a tensile Ge QW gain calculation. As discussed earlier, the barriers don't form a perfectly infinite step. Thus, the calculations of the wavefunction and the eigen energies need to consider a finite quantum well correction to the calculation. This will impact the emission wavelength as well as the gain through the transition matrix element in Eq 5.3.6. The impact of the infinite QW assumption on the wavefunctions of the electrons and holes is highlighted in **Figure 52**. The conduction band offset CBO and valance band offset VBO is highlighted. The transcendental equations for the finite QW is solved taking into account the varying band offset with tensile strain.

The physics necessary to evaluate the gain of a tensile strained Ge QW laser with a focus on the active region is complete at this point. The terms and physical considerations necessary to

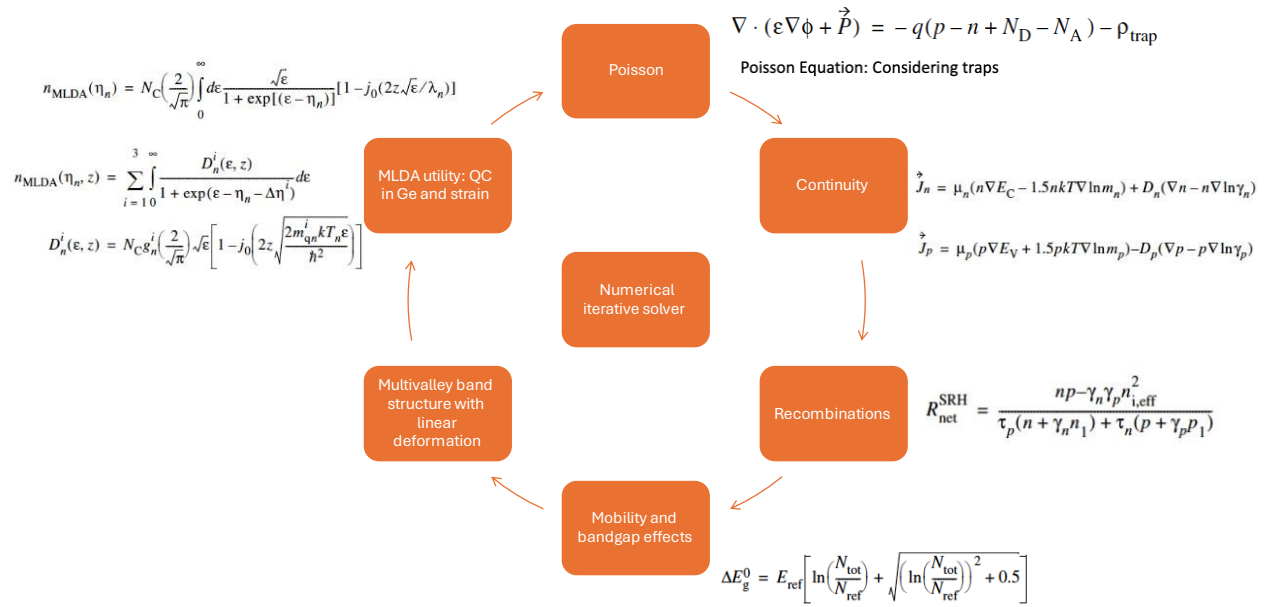


Figure 53. A brief description showing the various physical equations solved self-consistently within the TCAD numerical solver framework. Some key physical equations are illustrated.

evaluate Eq 5.3.5 are described, and now a brief outlook on the numerical computation framework is provided here. Sentaurus TCAD [7] is used to simulate the electrical, multi-valley and quantum corrected physical phenomenon in the 3D laser structure. Some of the ideal and non-ideal physical phenomenon included in the model are summarized in **Figure 53**. This electrical behavior is calibrated with experimental data for electrical transport devices such as FinFETs and NSFETs (Chapter 3 and 4). This provides a good degree of confidence on the Fermi levels, carrier densities, current densities, and recombination rates computed by this computation framework for the Ge

QW laser structure. More details on the TCAD framework [7] are provided in Chapter 2. Beyond calibrating the electrical quantum corrected phenomenon in this structure, one needs to feed in two key unknowns. These unknowns are conduction and valance band offsets for the tensile Ge on InGaAs QW and the minority carrier lifetime. Both of them need to be measured experimentally for multiple samples as a function of tensile strain. The band alignment and the band offsets are measured using XPS, whereas the minority carrier lifetime is measured using PCD. The details are discussed later in this chapter. The band alignment and the minority carrier lifetime are used to calibrate the TCAD models further. The minority carrier lifetime measured using PCD and the band alignment for tunable ε -Ge/In_xGa_{1-x}As systems are provided as input to the TCAD simulation suite [7]. This simulation framework considers a 3D numerical solver accounting for the drift-diffusion and quantum-corrected physics within the ε -Ge/In_xGa_{1-x}As QW structure. The model includes experimentally calibrated band offsets considering multivalley band structure and accounts for composition, strain, electric field, non-parabolicity, doping-dependent band structure, mobility, and effective mass. The electrical parameters such as electrostatic potential, quasi-fermi energy levels, current and voltage, recombination rates (SRH, Auger, and Radiative), band occupations, wavefunctions, and 6×6 $\mathbf{k} \cdot \mathbf{p}$ band structure are self-consistently solved [7] to calculate the optical gain spectra. The model also accounts for the thermionic emission rates over the heterointerfaces and a high ($5 \times 10^{12} \text{ cm}^{-2} \text{ V}^{-1}$) interface trap density at the two ε -Ge/In_xGa_{1-x}As heterointerfaces to ensure a more realistic electrostatic profile in the ε -Ge QW. The electrical parameters listed above are fed to TCAD laser-gain solver to calculate the optical gain of the ε -Ge/In_xGa_{1-x}As finite QW laser structure [1-3] TCAD computed metrics such as fermi levels, current densities, recombination rates *etc.* are consequently fed to a custom-made optical gain solver incorporating the laser gain physics discussed here in Chapter 5. The next sections move on to specific results of the Ge/InGaAs QW material system and the SCH waveguide in terms of design consideration, tunability and metrics.

5.4 Explorations of Ge based light sources: Challenges and Opportunities

Before moving on to lasing and SCH QW laser design specific for Ge, a brief review of the recent progress in lasing from Ge is provided. Lasing from indirect bandgap Ge has been a research endeavor for the past decade owing to the compatibility with Si technologies and emission ~ 1550 nm which is relevant for optical communication. The lower effective masses of Ge compared to GaAs and the pseudo-direct bandgap which is tunable using strain and alloying with Sn make it an attractive candidate for QW lasers. The challenge in achieving lasing from Ge is the dominant indirect L-valley which attracts large carrier populations but supports no radiative recombination, and techniques such as tensile strain and n-type doping have been suggested to lower the direct valley and achieve efficient lasing at lower threshold currents. One of the first reports for bulk Ge lasing included modeling the absorption spectra for heavily n-doped 200 nm thick Ge [8]. Using Ge with n-doping approaching $\sim 10^{20}$ cm $^{-3}$, and a tensile strain of 0.25 % attributed to the thermal expansion coefficient difference between Ge and Si, Liu *et. al.*, predicted that the threshold current could be lowered down to ~ 6 kA/cm ^{2} [8]. A similar approach of high doping and small tensile strain has been adopted in Ref. [9] to demonstrate the first lasing report from a Ge/Si cavity with a threshold current density approaching 300 kA/cm ^{2} . This approach has a few challenges; (i) the high n-type doping although helps raise the electron quasi-fermi energy closer to the direct band edge, results in aggravated Auger recombination, (ii) the material quality of Ge lasing media grown on Si substrate is defective due to the large lattice mismatch causing increased non-radiative recombination, (iii) considering the many-body effects, the band re-normalization at higher n-type doping can counter-act the fermi separation advantage provided by the high doping [10, 11] (iv) the cavity of a double heterostructure (DH) or QW needs to be Type I (with respect to direct bands) to provide confinement of carriers and optical field, the Si/Ge/SiGe system cannot provide this unless one relies on random defects at the interface to alter the band alignment [12]. Furthermore, it has been observed that the Ge-Si systems provide luminescence through indirect transitions between Δ -valleys in Si and holes in Ge resulting in an inefficient radiative recombination [13]. Kurdi *et. al.*, utilized a 30-band $\mathbf{k}\cdot\mathbf{p}$ calculation model to establish the material gain of ~ 3000 cm $^{-1}$ for FCA of 120 cm $^{-1}$ for bulk Ge with a tensile strain of 3 %. The optical transitions were neglected for the indirect L-valley, but the effect of the indirect valleys on the quasi-fermi energy movement and carrier conduction was considered [14]. Jiang *et. al.*

predicted a gain of $\sim 2000 \text{ cm}^{-1}$ for a 4 % uniaxial tensile strained Ge/SiGe QW system using 8 band $\mathbf{k}\cdot\mathbf{p}$. It was noted that uniaxial tensile strain results in TE dominant gain, unlike the biaxial tensile case where the polarization is TM [15].

Ge 7 nm QW cavity design and gain analysis for a Type I system with a SiGeSn barrier was modeled using first-principles calculations for a tensile strain of 2.7 % [5] and 0.5 % [16]. At a tensile strain of 2.7 % (corresponding to $\text{In} = 40 \%$), the Ge is a direct bandgap active region, and a significant density of carriers occupy the Γ -valley with the LH band being the dominant VB and hence the dominant mode is TM. This Ge-SiGeSn system has some key differences with the present work such as; only 1 LH bound state and no HH bound state, low band offset of 80-100 meV, and, a drastically higher refractive index of SiGeSn compared to InGaAs.

Another popular technique for making Ge transition to a direct bandgap material is alloying with Sn, with the transition occurring in the range $\text{Sn} \sim 7\text{-}10 \%$ [4, 10, 17, 18]. Chang *et. al.*, proposed a GeSn MQW with a SiGeSn cavity and used compressive strain (upward movement of HH) to potentially reduce the J_{TH} and make the dominant emission polarization TE. Furthermore, it was predicted that even when Ge is strongly direct bandgap at $\text{Sn} = 16 \%$, the direct band occupation is nearly 12 % which is slightly higher than tensile Ge. The TE material gain of $\sim 2500 \text{ cm}^{-1}$ was predicted at an emission wavelength of $2.8 \mu\text{m}$, and the net modal gain for the 5-MQW structure was $\sim 180 \text{ cm}^{-1}$ [4]. Fujisawa *et. al.*, used many-body theory (MBT) to circumvent the need for fitting parameters for broadening mechanisms generally associated with Fermi's Golden rule-based free carrier theory (FCT), to predict the lasing performance of MQW GeSn-SiGeSn Type I SCH system. The variation in spectral location and peak gain associated with the FCT as relaxation time is fitted can be avoided by using the MBT method. Peak material gain of $\sim 3000 \text{ cm}^{-1}$ was predicted at an emission wavelength of $2.9 \mu\text{m}$ for a 10 nm QW and band offsets in the range of 50-100 meV [10]. Mączko *et. al.*, utilized GeSn active layers and Ge barriers to form a QW laser structure with Type I alignment and band offsets in the range of 150 meV. The optimum Sn composition for forming the direct bandgap GeSn laser was determined to be 15 % where the emission is at $\sim 2.48 \mu\text{m}$. For narrow QW thickness as well as high Sn compositions, the material gain was seen to decrease because the carriers prefer to occupy L-valley in the Ge barrier rather than the GeSn direct valley, thus making thinner QWs unfavorable [18]. Dutt *et. al.*, used the empirical pseudopotential method and the absorption spectra relation to estimate lasing performance from 300 nm bulk GeSn-on-Si DH cavity (Type II alignment). The high n-type

doping requirement was reduced to $\sim 10^{17} \text{ cm}^{-3}$ using the Sn alloying and achieving a material gain of $\sim 1000 \text{ cm}^{-1}$ while reducing the J_{TH} to $\sim 2.4 \text{ kA/cm}^2$, a number comparable to typical direct bandgap lasers. Unlike the tensile Ge case, the GeSn spectra has TE polarized emission due to the degenerate LH and HH bands [17]. Lasing from GeSn cavities was experimentally demonstrated by Wirths *et. al.*, using optical pumping and temperature-dependent PL measurements. The gain comparable to direct bandgap lasers of $\sim 100 \text{ cm}^{-1}$ was achieved while a transition to direct bandgap GeSn was found to be $\sim 9 \%$ and a lasing threshold of $\sim 300 \text{ kW/cm}^2$ [6].

Photoluminescence (PL) measurements can provide a good estimate of the lasing performance of materials before the semiconductor fabrication of devices, which is usually a destructive process [19-21] Nam *et. al.*, demonstrated PL as a function of uniaxial strain and temperature in a Ge microbridge. The broken degeneracy of the LH and HH bands and the corresponding difference in intensity attributed to the difference in DOS is visible at high strain in the form of two distinct fitted peaks. The polarization at higher emission wavelength (higher strain) is seen to be dominated by the valley with low DOS and the polarization is perpendicular to the strain axis [19]. Fei *et. al.*, proposed a Ge/SiGe MQW structure and showed through PL measurements that the direct transitions are indeed enhanced compared to bulk Ge due to the confinement of wavefunctions in the Ge QW structure [20]. Due to the reduced lasing efficiency in Ge/SiGe QW structures attributed to the compressive strain, Chen *et. al.*, proposed the use of external tensile strain using SiN stressors (characterized using PL and Raman measurements) to compensate and make the active layer tensile strained [22]. The biaxial tensile strain increased with increasing SiN stressor thickness, and a clear shift was observed in the PL spectra to higher wavelengths while maintaining the same intensity. It is, however, unclear why the TE gain was found to be significantly higher than the TM gain after application of biaxial tensile strain considering the HH-LH split, and why the gain increased with tensile strain even though the PL intensity was the same [22].

A detailed comparison of various explorations of Ge-based light-emitting devices and materials over the years is provided in **Table III**. Important metrics of typical lasing devices are compared to the proposed tensile strained Ge laser discussed in this work in this section. The detailed structure, composition, growth, metrics, performance trends, and design considerations shown here are elaborated on in the following sections.

TABLE III : Benchmarking of the proposed monolithic ϵ -Ge/InGaAs SCH QW laser with electrically pumped Ge based lasers

Ref.	Lasing Material and Size	Type of Study	Technique	Cavity	Material Loss	JTH (kA/cm ²)	Gain (cm ⁻¹)	Band Alignment	Band Offsets (c, v) in eV	Emission Wavelength (nm)	Temperature and polarization
8	Bulk Ge 200 nm	Theory	N-doping $\sim 1e20$, tensile Ge 0.25 %	Ge-Si	$\sim 500^{**}$	5.8	400*	Type II	-	1550	-
9	Bulk Ge 100 nm	Exp	n-doping $\sim 1e20$, tensile Ge 0.25 %	poly-Ge-Si	-	~ 280	-	Type II	-	1650	-
5	Ge SQW 7 nm	Theory	Strain balanced, Tensile Ge 2.7 %	Ge-SiGeSn QW	-	-	$\sim 2300^{\#}$	Type I	$\sim 0.3, \sim 0.1$	~ 3100	300K, q-TM
16	Ge MQW 7 nm	Theory	Strain balanced, 5QW Tensile Ge 0.5 %	Ge-SiGeSn QW	$\sim 100-1000$	-	$\sim 3000^{\#}$	Type I	$\sim 0.08, \sim 0.06$	1550	300K, q-TM
4	GeSn QW 10 nm	Theory	Strain balanced, Sn = 16 %, 5QW Compressive 0.5 %	GeSn-SiGeSn QW	~ 1000	$\sim 10^{##}$	$\sim 800^{\#}$	Type I	$\sim 0.11, \sim 0.13$	2883	300K, q-TE
18 ***	GeSn QW 8 -14 nm	Theory	Sn = 10- 20 %, Compressive QW	GeSn- Ge QW	-	-	~ 1200	Type I	$\sim 0.17, \sim 0.16$	~ 2580	300K, q-TE
15	Ge QW	Theory	Uniaxial tensile 4 %, N-doping $1e19$	Ge-SiGe	400-600 **	-	~ 2000	Type I	$\sim 0.02, \sim 0.12$	~ 2210	300K, q-TE
14	Bulk Ge	Theory	High N-doping, tensile Ge 3 %	NA	120 **	-	~ 3000	-	-	~ 3000	80K
17	Bulk GeSn 300 nm	Theory	Moderate N-doping, Sn 0-10%	GeSn-Si	-	~ 2	~ 1200	Type II	-	~ 2500	-
13	Bulk Ge 350 nm	Theory	High N-doping, tensile Ge 0.25 %	Ge-SiGe	~ 517	$\sim 2-5$	3000*	Type II	-	1550	-
11	Bulk Ge	Theory	Doping, MBT	NA	$\sim 200-800$	$\sim 1-10$	~ 400	-	-	~ 1550	-
10	GeSn QW 10 nm	Theory	SCH compressive QW	GeSn-SiGeSn	$\sim 1000-2000$	-	~ 3000	Type I		~ 2900	-
<i>This work</i>											
Ge QW In = 16 %	ϵ -Ge/InGaAs QW 10 nm	Theory	SCH QW tensile, tunable design cavity	Ge-InGaAs	1935	10.7	3042	Type I	0.38,0.28	1799	300K, q-TM
Ge QW In = 24 %	ϵ -Ge/InGaAs QW 10 nm	Theory	SCH QW tensile, tunable design cavity	Ge-InGaAs	2202	3	3009	Type I	0.22,0.35	2137	300K, q-TM
Ge QW In = 30 %	ϵ -Ge/InGaAs QW 10 nm	Theory	SCH QW tensile, tunable design cavity	Ge-InGaAs	2475	2.4	2974	Type I	0.2,0.4	2500	300K, q-TM

* Net material gain, ** FCA, *** 12 nm QW with Sn = 15 %, $N_{inj} = 6e18$, $\# N_{inj} = 4e12$, ## assuming efficiency of 75 %

5.5 Impact of tensile strain on band structure and band offsets of Ge

The band offsets for the tensile Ge on InGaAs QW structure are measured and used to calibrate the band alignment calculations within TCAD to ensure accurate prediction of band properties. The band alignment of various In compositions in ε -Ge/In_xGa_{1-x}As heterostructures were constructed using the experimentally determined band offset values measured using the x-ray photoelectron spectroscopy (XPS) on a PHI Quantera SXM-03 (Scanning XPS Microprobe) system, reported in Refs. [23-25]. For the band structure and offsets calibration, the 30×30 **k·p** calculated material and band parameters are adopted from Ref. [14]. The simulations are tuned to utilize a 6×6 **k·p** approximation along with linear deformation theory within Sentaurus TCAD [7] to accurately predict experimental values of band offsets, and 30×30 **k·p** calculations of the band structure of ε -Ge/In_xGa_{1-x}As system. To ensure the accuracy of the electrical predictions, the drift-diffusion and quantum-corrected electrical behavior of the model for nanoscale devices have been calibrated and presented in Chapters 3 and 4.

First, the impact of tensile strain on the band structure of Ge is discussed. The 4 important bands in Ge are the CBs L- and Γ -valley, and the VBs LH and HH-bands. **Figure 54** shows the

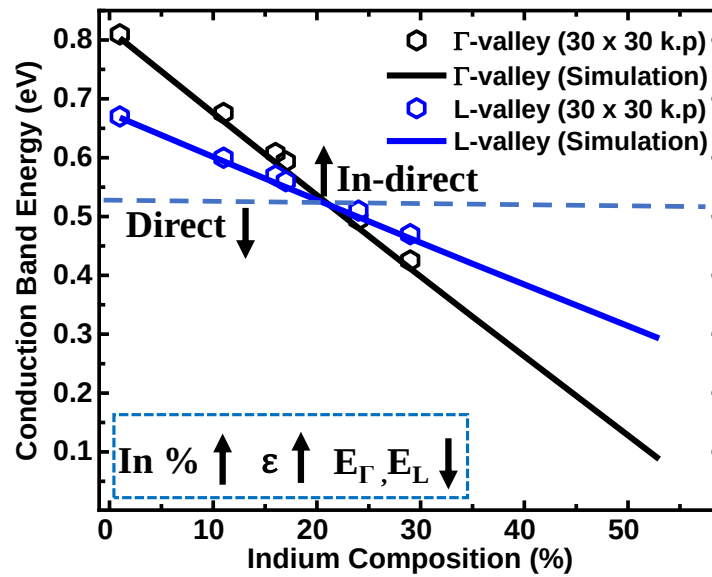


Figure 54. Impact of tensile strain applied on the Ge QW via variation in the In composition in the underlying InGaAs. A comparison of 30x30 **k.p** with the simulation framework is shown to illustrate the validity of the models.

conduction band energy of ϵ -Ge due to L-and Γ -valley as a function of In compositions by 30×30 $\mathbf{k} \cdot \mathbf{p}$ and TCAD simulation model [7]. In this figure, the open circle is the data obtained from 30×30 $\mathbf{k} \cdot \mathbf{p}$ for both L-and Γ -valley, and the solid line represents the simulated data with TCAD. It can be noted that the tensile strain lowers the Γ -valley faster than the L-valley. Increasing the In composition in InGaAs results in a higher tensile strain in Ge. The cross-over point between the L-and Γ -valley is the point where Ge transitions to a direct band gap material. The indirect-to-direct bandgap transition takes place $\sim 24\%$ In ($\epsilon = 1.6\%$), reaffirming the finding reported in Ref. [2,5]. One can note a general trend that the increasing tensile strain results in a large red-shifting of both the band gaps for Ge. Although the L-valley does not participate in radiative transitions thus no gain production is possible, it is important to capture the deformation of the L-valley

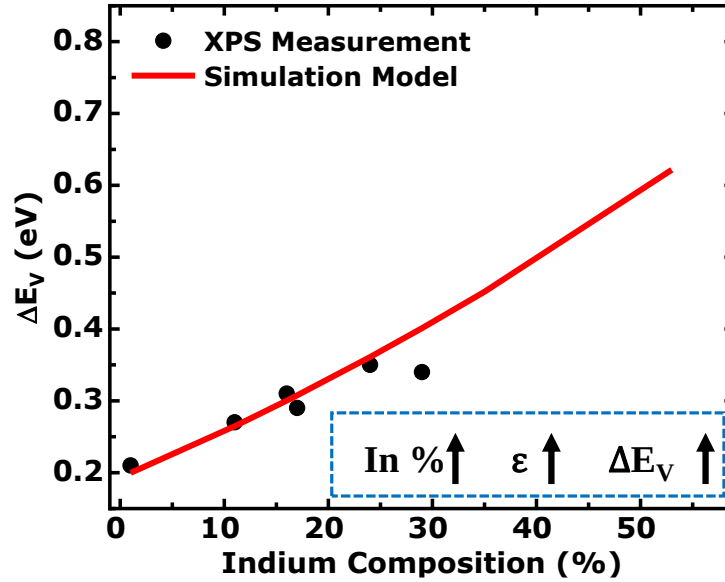


Figure 55. Experimentally measured valence band offset for various samples with different In composition. The measurement is done using XPS to illustrate the impact of increasing tensile strain on the valence band offsets.

accurately. The L-valley has a very large DOS resulting in a very large impact on the electrical conduction of the Ge layer, carrier occupations in various bands as well as mobility. Thus, ensuring that the L-valley is also appropriately included in the models ensures the electrical as well as optical validity of the model.

Figure 55 shows the experimentally measured and simulated valence band offsets (ΔE_v) of ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ heterostructures as a function of In composition in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer. The

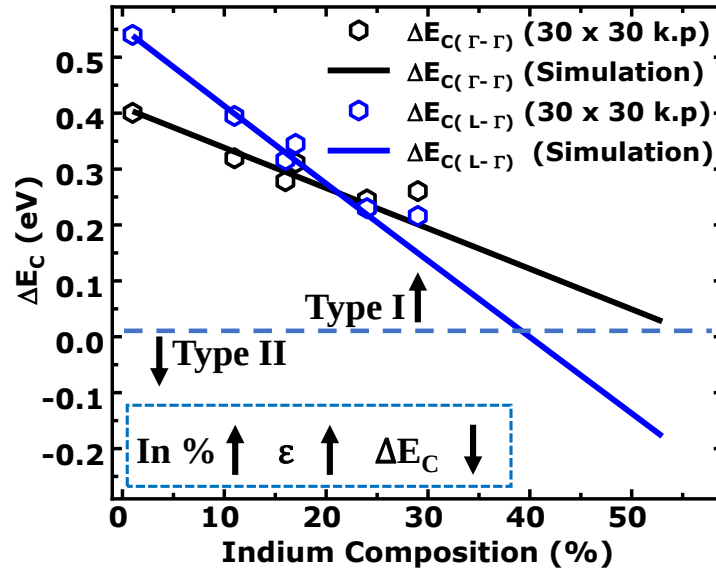


Figure 56. The conduction band offset as a function of In composition and correspondingly the tensile strain in Ge. Calculated based on VBO measurements shown earlier. The transition from type I to type II is shown.

solid circle represents the experimental data and the solid line is the simulated data, and an excellent agreement can be seen between the experimental and modeled band offsets. In addition, using the measured value of ΔE_v and bandgap values of both ϵ -Ge as well as $\text{In}_x\text{Ga}_{1-x}\text{As}$ via $30 \times 30 \text{ k}\cdot\text{p}$ [14, 26], the conduction band offsets (ΔE_c) are evaluated. Due to the two conduction band minima (L- and Γ -valley), one can construct ΔE_c using Γ -valley of $\text{In}_x\text{Ga}_{1-x}\text{As}$ (Γ -valley dominates for any In composition) and either L-valley or Γ -valley of Ge depending on the strain present within the ϵ -Ge layer (via $\text{In}_x\text{Ga}_{1-x}\text{As}$ strain template). **Figure 56** shows the ΔE_c using the bandgaps of ϵ -Ge and $\text{In}_x\text{Ga}_{1-x}\text{As}$ as a function of In composition between the L- and Γ -valley of ϵ -Ge and Γ -valley of $\text{In}_x\text{Ga}_{1-x}\text{As}$, shown earlier. The open circle is the data obtained from $30 \times 30 \text{ k}\cdot\text{p}$ and solid lines from the simulated results fitted to the $30 \times 30 \text{ k}\cdot\text{p}$ data. The conduction band offset is calculated using the simple relation $\Delta E_c = \Delta E_g - \Delta E_v$, where the term ΔE_g is the difference in the well-known bandgaps of Ge and InGaAs at the particular tensile strain and In composition, and ΔE_v is the valence band offset discussed earlier. In all cases, there is an excellent agreement between the experimental and the simulated results, essential for making predictions about the quantum well, electrical injection, and gain/emission.

These results for the band energies, offsets, and lineup show that as the In composition increases in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer, the tensile strain in the Ge QW increases resulting in

- (i) a decrease in Γ -valley of Ge at a rate of $13.24 \frac{meV}{In \%}$ or $196.02 \frac{meV}{\epsilon \%}$, and
- (ii) a decrease in L-valley of Ge at a rate of $6.89 \frac{meV}{In \%}$ or $102.02 \frac{meV}{\epsilon \%}$.

Furthermore, the tensile strain results in a broken degeneracy between light hole (LH) and heavy hole (HH) valence bands, while moving the LH band upwards. It is important to note that radiative transitions are possible from the LH as well as the HH bands, and the carriers participating in these transitions will experience different band offsets as well as different transition energies, optical polarization, and gain.

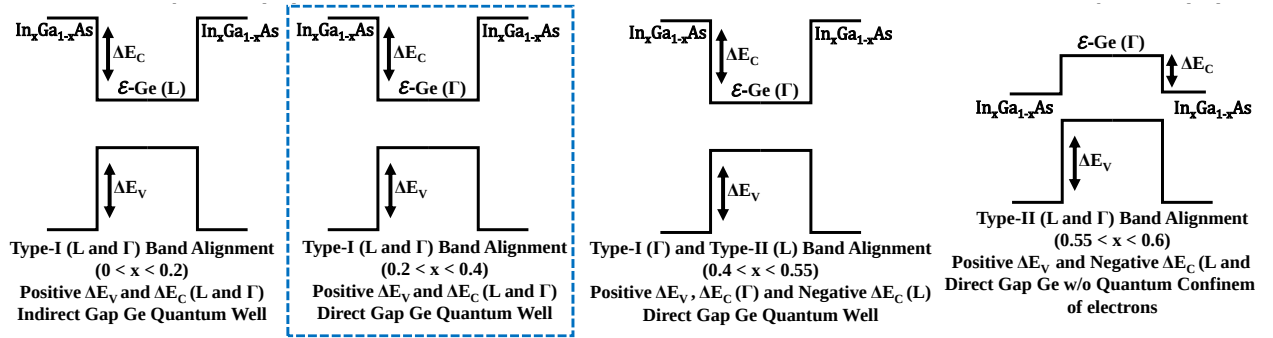


Figure 57. The various regimes of band alignment and direct-ness for different In compositions and corresponding tensile strains for the InGaAs-Ge-InGaAs QW.

Figure 57 shows the different band alignment configurations for $In_xGa_{1-x}As/\epsilon\text{-Ge}/In_xGa_{1-x}As$ QW configuration as a function of In compositions. Here, we assume symmetric heterointerface band alignment of $In_xGa_{1-x}As/\epsilon\text{-Ge}$ QW configuration. The band alignment remains type I up to 40 % In composition for L-valley and 55 % In composition for Γ -valley. For In compositions $0.4 < x < 0.55$ range, the band alignment is type I with Γ -valley of $\epsilon\text{-Ge}$ (the band alignment is Type-II for the L-valley of $\epsilon\text{-Ge}$) thus ensuring acceptable direct bandgap QW confinement up to In composition of $\sim 55\%$. The system transitions to a type II alignment for both L- and Γ -valleys beyond an In composition of $\sim 55\%$. The bandgap of $\epsilon\text{-Ge}$ drops significantly for high tensile strain and beyond an In composition of 60 %, the Ge bandgap is negative. It can also be seen that the $\epsilon\text{-Ge}/In_xGa_{1-x}As$ QW system will remain type I for the majority of the In compositions (0 - 55 %) and completely type II for a short range (55 - 60%). This ensures that the $\epsilon\text{-Ge}$ QW provides carrier confinement and has the potential to be a tunable light source over a wide range of wavelengths.

XPS measurements provide information about the valence band maximum (VBM), which is always aligned with the LH band for all strain configurations studied here, thus the offsets and energies shown above correspond to the LH band. The HH-band energies and offsets can be calculated as a function of In composition or strain relative to the LH band as follows, $E_{VBM,HH} = E_{VBM,LH} - (8.66 \text{ meV} \times \text{In } \%)$. Due to the difference in the behavior of the LH and HH bands with applied tensile strain, the carriers in the HH band experience a small and constant valance band offset in the range of 0.15 - 0.19 eV, unlike the LH band which can be seen to vary considerably in **Figure 55**. Due to the faster reduction rate of the Γ -valley compared to the L-valley with increasing In composition, Ge transitions to a direct bandgap active material at In composition of $\sim 24 \%$ and corresponding tensile strain of $\sim 1.6 \%$. In the ϵ -Ge QW laser, the band alignment between the ϵ -Ge active layer and the $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide layer, determines the extent

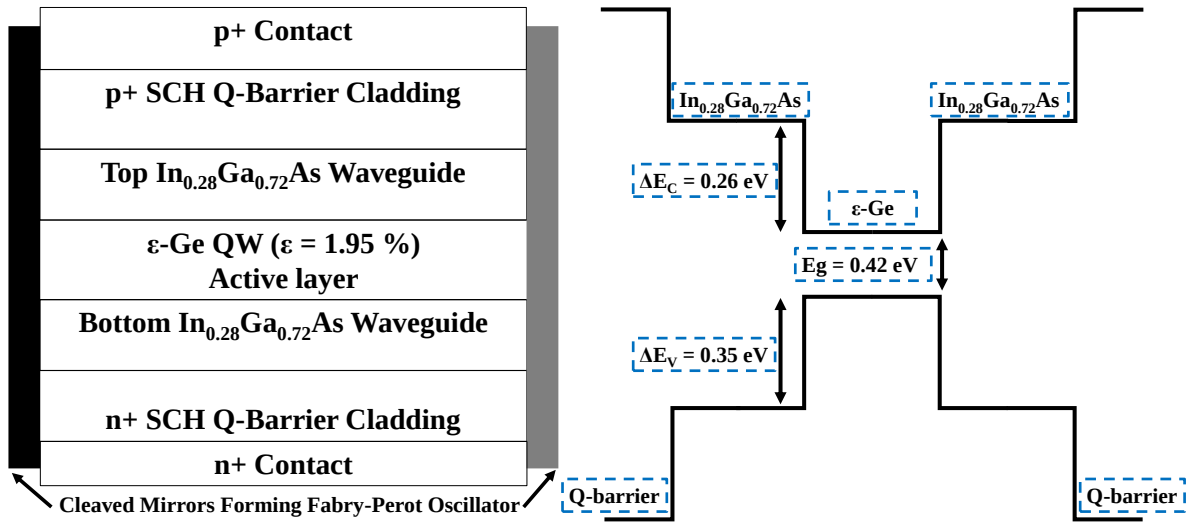


Figure 58. Schematic of the proposed 1.95 % tensile strained Ge/InGaAs SCH QW (left) and band alignment (right). Schematic of the proposed 1.95 % tensile strained Ge/InGaAs SCH QW (left) and band alignment (right).

of quantum confinement of both electrons and holes. This also affects the overlap between the electron and hole wavefunctions as well as wavefunction spillage outside the QW for higher In compositions. Furthermore, as Ge transitions from an indirect bandgap material to a direct bandgap material, the band alignment also gradually changes, as seen in **Figure 57**. The ΔE_v determines the confinement of holes in the ϵ -Ge active layer, and it is measured to be always positive, indicating that hole bound states will exist for all In compositions and corresponding

tensile strains in Ge. Due to the significantly higher density-of-states (DOS) in the Ge L-valley ($\sim 50\times$) compared to the Γ -valley [2], the carrier occupations in the L-valley are dominant even after Ge transitions to a direct bandgap lasing medium. Thus, the band alignment associated with the L- and Γ -valley needs to be considered simultaneously to understand the complete 3D electrical behavior of the ε -Ge QW laser. However, radiative transitions are only possible from the Γ -valley since the L-valley transition probability is extremely low, contributing negligible gain [8]. Finally, using the band offset and band deformations measured and modeled in this section, one configuration of the Ge QW laser is chosen and highlighted in **Figure 58**.

5.6 Minority carrier lifetime measurement: μ -PCD for tensile Ge/InGaAs

Minority carrier lifetime and band alignment are key attributes of a QW laser. These attributes are measured using microwave photoconductive decay (PCD) and x-ray photoelectron spectroscopy (as a function of In composition), respectively. The band offsets and alignment as a function of In composition, calibration of the data to the model as well as the incorporation of the band deformations into the model were discussed in the previous section. Here we briefly describe the lifetime measurements for tensile Ge QW samples. The direct growth of Ge on Si, although an attractive solution for large-scale manufacturing, suffers from a large lattice mismatch ($\sim 4\%$), resulting in defects and dislocations during epitaxial growth [27]. This degradation in epitaxial Ge material quality can be inferred from the minority carrier recombination lifetime measured through the microwave reflection photoconductive decay (μ -PCD) method [28]. A higher carrier lifetime is an essential attribute of a bulk or quantum well light source, as it determines the efficiency of electrical conversion as well as the performance of the laser [28, 29]. The primary hurdle in the development of an efficient on-chip Ge-based light source is the material quality, i.e., the minority carrier lifetime [29]. The GaAs-based material system (*i.e.*, using $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ based intermediary buffers/barriers with GaAs substrate) is a solution for growing high-quality epitaxial Ge for two key reasons: (i) lattice match between the epitaxial Ge layer and the GaAs substrate resulting in lower defect density, and (ii) transferability of GaAs based growth and process recipes to large area cost-effective, Si substrate.

Minority carrier lifetimes of each tensile Ge epitaxial layer were measured using μ -PCD technique at the laser excitation wavelength of 1500 nm ($E_{\text{ph}} \approx 0.83$ eV) which excites the electrons from the valence band to both L- and Γ -valleys of the conduction band. The μ -PCD measurement was carried out at the National Renewable Energy Laboratory. Wherein, the top of each sample surface was irradiated by a laser source with 10 pulses per second (pulse width = 5 ns) at 1.8 mW to 18 mW for 1500 nm excitation wavelengths. The measurement setup is such that a sample is placed beneath a rectangular waveguide (WR-42, dimension: ~ 4.3 mm $\times$ 10.7 mm) that guides a 20 GHz microwave signal to reflect from the sample surface while it is irradiated by the laser source from the top. Allowing 3 ns for the generated carriers to diffuse away from the sample surface after this laser excitation, the intensity of the guided microwave reflected signal from the sample surface was recorded to monitor its decay as μ -PCD signal. This is correlated to the excess

carrier density that maps the photoconductivity changes in the sample. Through this μ -PCD technique, minority carrier lifetimes of the tensile Ge epitaxial layers were extracted using a single exponential decay curve-fit function. The effective minority carrier lifetime referred to here is obtained after the initial surface recombination-related decay, also called the short lifetime component region; details of the extraction technique are explained elsewhere [28].

The photogenerated carriers undergo surface states induced carrier recombination prior to their diffusion (deeper) into the bulk-like epitaxial region of the sample. The higher energy photons (here, 1500 nm) have stronger absorption, and this photoexcitation leads to a different initial excess carrier distribution where more carriers are generated near the surface. This would lead to more surface recombination and a decay curve more dominated by the initial steep decay. The rate of diffusion towards the bulk region is impacted by the excess carriers remaining after the initial surface recombination, i.e., high surface recombination is related to a high diffusion rate, which gives rise to low minority carrier lifetimes. The minority carrier lifetimes were extracted from the μ -PCD versus time decay curve by fitting the curve to the single exponential decay function, after the initial surface recombination related fast decay component $V_{0,pcd} = V_0 e^{-\frac{t}{\tau_m}}$, where τ_m is the minority carrier lifetime and V_0 is a constant related to the μ -PCD signal's peak intensity. A carrier lifetime value extracted from deep into the μ -PCD signal intensity represents the bulk carrier lifetime, which is higher than an effective carrier lifetime that takes into account the initial decay and diffusion from the near surface region of the sample.

The prediction of ε -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW laser performance requires an assessment of Ge active layer material quality, to qualitatively affirm low defects and dislocations. Defects and dislocations become centers of non-radiative recombination resulting in a poor IQE. The carrier lifetime of $\sim 0.7\%$ ε -Ge/ $\text{In}_{0.11}\text{Ga}_{0.89}\text{As}$ heterostructure and the 1.95% ε -Ge samples were evaluated using a 1500 nm laser wavelength using microwave photoconductive decay (μ -PCD) measurement technique, shown in **Figure 59**. The estimated injected carrier density is approximately 10^{13} cm^{-3} and the excitation power was $\sim 2 \text{ mW}$, details of μ -PCD measurement technique can be found in Ref. [27]. The minority carrier recombination lifetime of 81 ns for 0.7% ε -Ge and 64ns for the 1.95% ε -Ge samples due to Shockley-Read-Hall (SRH) recombination was determined by fitting the μ -PCD decay curve. This PCD lifetime value for the SRH recombination, as well as other non-

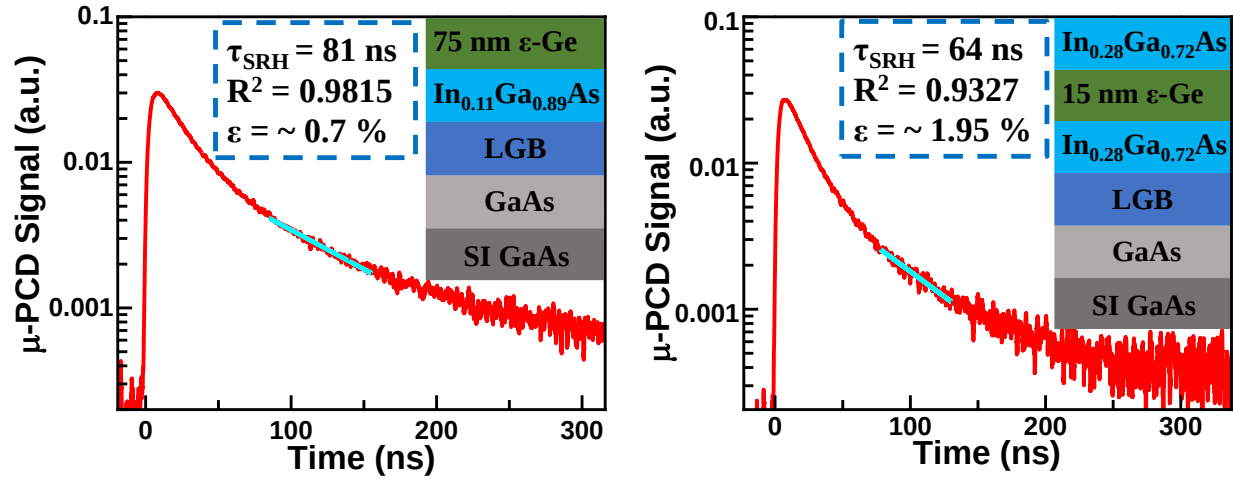


Figure 59. The minority carrier lifetime measured using microwave PCD signal decay measurement for two samples of tensile strained Ge on InGaAs, (left) 0.7 % and (right) 1.95 %. The fitting quality is ensured to be approaching 1.

radiative recombination mechanisms such as Auger processes, are included in the calibrated model. The internal quantum efficiency (IQE or η_i) is the ratio of radiative recombination rate to the total recombination in the ϵ -Ge QW laser structure at maximum gain, $\eta_i = \frac{J_{rad}}{J_{rad} + J_{non-rad}}$, where $J_{non-rad}$ includes the non-radiative recombination mechanisms such as SRH and Auger recombination [7], both of which are dependent on the band structure, minority carrier lifetime, and injection density.

In conclusion, these experimentally determined attributes of a ϵ -Ge QW laser design such as structure, tensile strain, band alignment, and minority carrier lifetime define the critical design metrics of the laser *i.e.*, emission wavelength, internal quantum efficiency (IQE), threshold current density (J_{TH}), power consumption, optical confinement, electrical confinement of the electron and hole wavefunctions, wavefunction overlap, polarization, and maximum optical gain, in an interdependent manner. Here, we isolate the effects of these design parameters on the performance of a ϵ -Ge QW laser and quantify the design space where Ge can be an efficient coherent light source.

5.7 Tensile Ge QW SCH laser: Structure and Adaptive Waveguide design

After reviewing the quantum well gain calculation, tensile Ge band properties, Ge-InGaAs band alignment and explorations in literature, the proposed Ge QW laser structure as a part of this work is shown in **Figure 60**. The band structure on the left side has the Ge QW surrounded by InGaAs composition-controlled layers. The detailed analysis of a Ge QW is discussed earlier in this section. The change in the band offsets due to the change in the In composition, as discussed earlier will affect the band alignment. These InGaAs layers, along with forming the potential well to confine the electron and hole wavefunctions, also form the waveguide where the optical field travels and amplifies during the lasing operation. The outermost layers, on the top and bottom sides, are the cladding layers formed with the quaternary alloy AlGaInAs. These layers provide a large band offset thus confining the optical field within the waveguide. The outermost layers are also responsible for providing carriers, electrons, and holes into the laser cavity through the

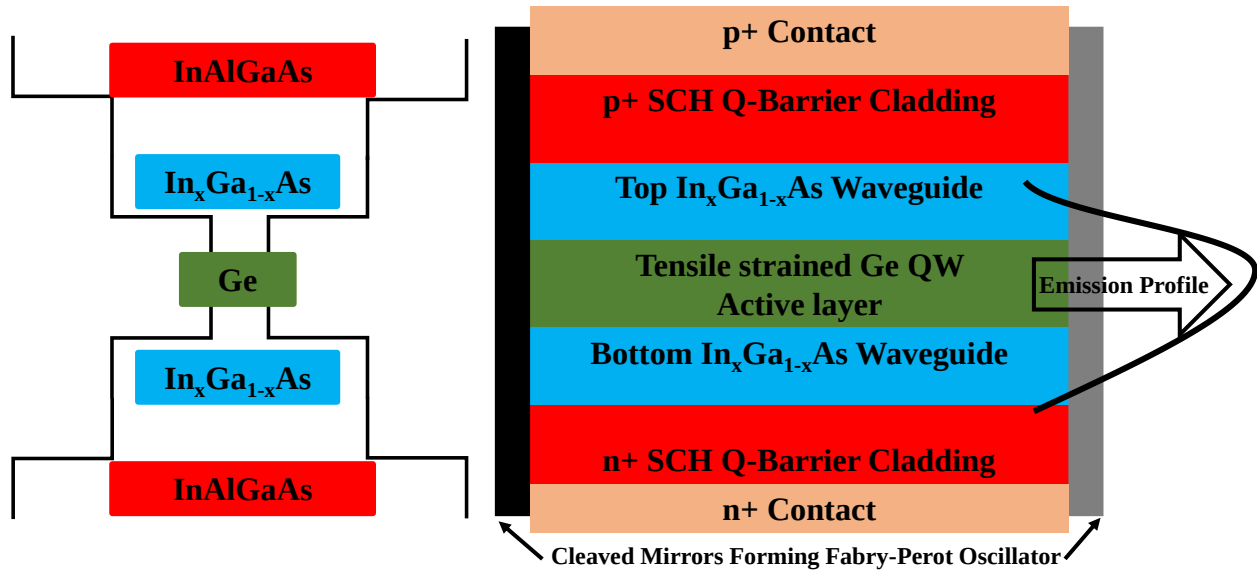


Figure 60. Schematic of the SCH Ge-on-InGaAs quantum well laser structure (right) and corresponding band structure (left), utilizing pseudomorphic monolithic growth. The entire structure can be grown monolithically on a GaAs substrate.

electrical terminal contacts, hence these layers are heavily doped. Mirrors on each side in the orthogonal direction, often formed through the cleaving of the wafer, are present to form the Fabry-Perot oscillator amplifying the optical field within the laser cavity.

The ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW structure shown in **Figure 60** can be grown on a GaAs substrate followed by a lattice grading $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer to mitigate the lattice mismatch-induced defects and dislocations. The topmost part of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer forms a virtually defect-free bottom waveguide layer for the ϵ -Ge QW structure. The pseudomorphic growth of ϵ -Ge on $\text{In}_x\text{Ga}_{1-x}\text{As}$ is possible [30], provided the thickness of the ϵ -Ge epitaxial layer remains below the critical layer thickness [31]. The AlGaInAs quaternary separate confinement heterostructure (SCH) layer can be grown before the InGaAs bottom waveguide layer with p -type doping and after the InGaAs top waveguide layer with n -type doping. Recently, 6 Å interface abruptness of ϵ -Ge/ $\text{In}_{0.24}\text{Ga}_{0.76}\text{As}$ heterostructure (grown by MBE) was demonstrated by atom probe tomography [30]. Thus, such growth of a multilayer heterostructure, which can form a ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW laser is possible with minimal defects and dislocations in the active region.

Compositionally graded buffers that utilize the benefits of metamorphic as well as pseudomorphic growth are of great interest since they offer an approach to bridge the substrate lattice constant to a desired value for device applications such as high electron mobility transistors or QW lasers. The growth of high quality ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW structures is achieved through vacuum interconnected dual chamber solid source molecular beam epitaxy [30]. A separate confinement layer based on a quaternary alloy, AlGaInAs (cladding layer) is needed for optical confinement while also providing the carriers for injection into the QW. One way to achieve this is to introduce the Al atoms into the InGaAs during material synthesis, forming a quaternary AlGaInAs layer. The choice of the quaternary AlGaInAs composition requires consideration of a key trade-off between growth ease and optical confinement of the emission electric field. Using a higher composition of Al needs a higher growth temperature and higher Al results in more surface undulations and roughness. Whereas, a higher Al composition would result in a higher bandgap of the quaternary, thus providing a higher refractive index difference with the QW, consequently better optical confinement. However, using a low Al composition reduces the bandgap and refractive index differences between the waveguide core and the cladding, thus reducing the optical confinement. Furthermore, the In composition in the quaternary buffers (Q-buffers) needs to be identical to the In composition in the confinement layer ($\text{In}_x\text{Ga}_{1-x}\text{As}$) of the QW during MBE growth, thus providing a constraint on the choice of the Q-buffer composition.

The emission profile of the optical field generated by recombinations in the Ge QW need to be confined in the waveguide. Thus a refractive index step between the InGaAs waveguide

layers and the SCH cladding is necessary. The confinement of the optical mode depends on the refractive index difference between the AlGaInAs SCH cladding, InGaAs waveguide, and ϵ -Ge QW active region as well as the emission wavelength (function of In composition and tensile strain), geometry, and composition. The optical confinement factor Γ_{opt} , (not to be confused with the Γ -valley, discussed above), needs to be determined for every configuration of emission profile to maintain optimum confinement of the optical mode. It is calculated considering a step refractive index with $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide core and $(\text{AlGa})_{1-x}\text{In}_x\text{As}$ SCH Q-barrier (refractive index is assumed to be 3.1) as the cladding. The refractive index (n_1) and bandgap of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide core are calculated according to the Sellmeier equation [32], where the lasing wavelength is obtained from the gain spectrum of the ϵ -Ge QW laser. The optical confinement factor (Γ_{opt}) is calculated assuming a 3-layer symmetric waveguide confining the mode as shown schematically using the emission profile in **Figure 60**, forming the characteristic equation given by $k_z \tan\left(\frac{k_z d}{2}\right) = \gamma$ where k_z is the propagation constant in the active region along the growth direction (z-axis), d is the total thickness of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide, γ is the propagation constant for the cladding Q-barrier layer (AlGaInAs) with $k_z^2 + \gamma^2 = k_0^2 (n_1^2 - n_2^2)$ and k_0 as the free space wave-number [1, 2]. The fraction of the electric field contained in the central slab of the waveguide can be calculated using the relation [1, 2],

$$\Gamma_{opt} = \frac{\int_{-d/2}^{d/2} |E(x, z)|^2 dz}{\int_{-\infty}^{\infty} |E(x, z)|^2 dz} = \frac{1 + (2\gamma d/V^2)}{1 + (2/\gamma d)}, \quad (5.6.1)$$

where, $V = k_0 d \sqrt{n_1^2 - n_2^2}$ is the normalized frequency and n_2 is the refractive index of the AlGaInAs SCH Q-barrier layer. The Ge QW thicknesses in the 5 - 20 nm range confined inside the $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide face an inverse relation for the optical confinement [3]. The optimum Γ_{opt} is found by maximizing these transcendental relations using iterative solutions. In addition, the overlap of the optical energy distribution with the QW needs to be maximized within the waveguide to obtain the maximum confinement factor (Γ_m). This confinement maxima (Γ_m) depends on the wavelength of emission, step-graded refractive index, QW thickness, and the thickness of the SCH layer. As the In composition in the waveguide is increased, the tensile strain in Ge and correspondingly the emission wavelength (λ_e) increases. Thus, the optimal waveguide

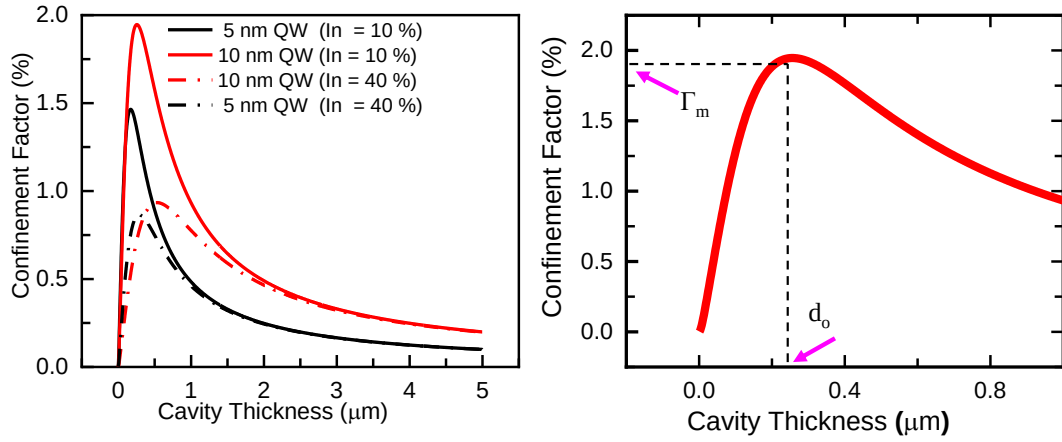


Figure 62. Determining the optimum optical confinement factor for different In composition, corresponding tensile strains and quantum well thicknesses.

design for different In composition and ϵ -Ge QW thickness is shown in **Figure 62**, indicating that for a particular In composition and ϵ -Ge QW thickness, there exists an optimal waveguide

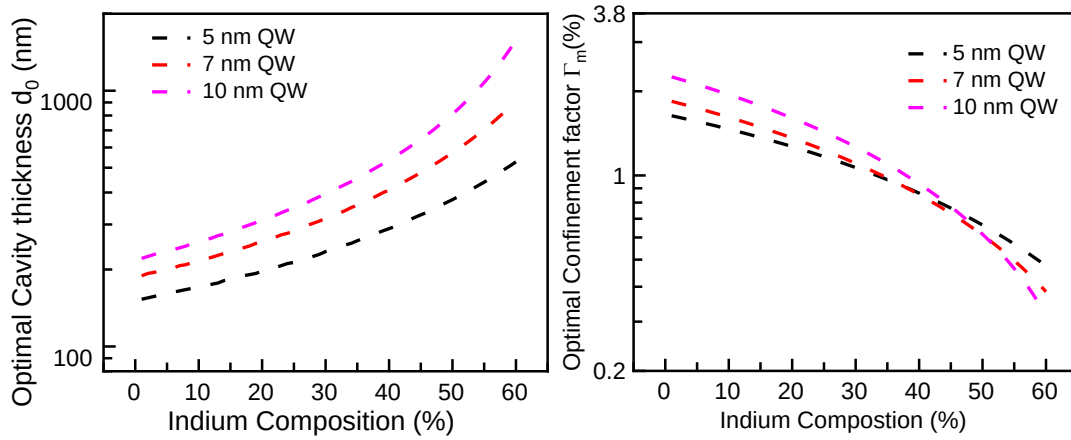


Figure 61. Using the adaptive design methodology to find the optimal cavity thickness for different quantum well thicknesses and In compositions (left), and the corresponding maximum optimum optical confinement factor attainable for the particular design configuration (right).

thickness d_o where the Γ_{opt} is optimal (Γ_m). The optimal design point is then the location of the peak as shown in **Figure 62**. The variation of d_o and Γ_m with In composition is shown in **Figure 61**. Further, detail contour plots for the optimum d_o and Γ_m covering a wide range of In compositions and quantum well thicknesses is shown in **Figure 63**. Optical confinement factors are expected to be nearly identical for the TE and TM modes for a fixed emission wavelength [1].

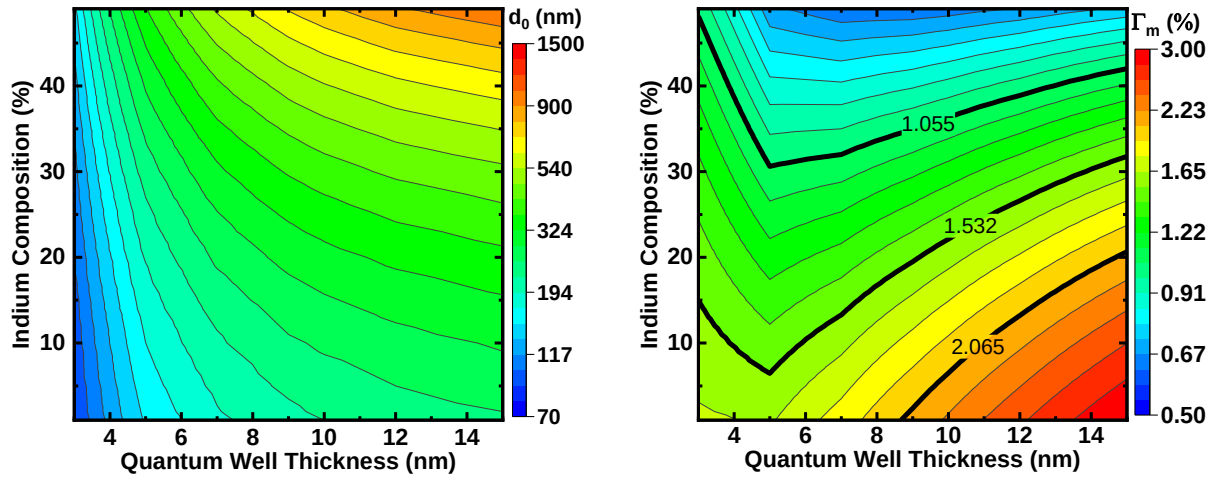


Figure 63. Variation of the optimum waveguide thickness (left), and optimal confinement factor (right) attainable with AD as a function of In composition and quantum well thickness.

But in the proposed ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW laser structure, the Γ_{opt} for the TE and TM modes would vary marginally depending on the emission wavelength of the LH and HH transitions, and correspondingly affect the gain and threshold performance.

For the results shown here, the waveguide cavity thickness, *i.e.*, the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer thickness on either side of the ϵ -Ge QW is fixed at the optimum value $d_0/2$ based on the Adaptive design (AD) depending on the QW thickness and In composition. This approach is well-suited for the gain and threshold predictions, where the Γ_{opt} for any design combination is ensured to be maximum. For certain regions in these results (*e.g.*, at In = 20 - 40%), one can notice that the

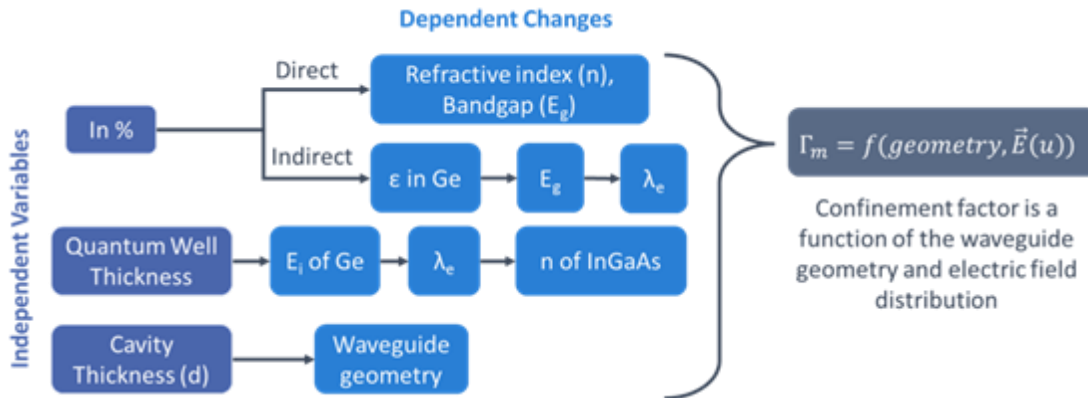


Figure 64. Summary of the interdependent impact of the design variables on the trnsile Ge QW laser performance, thus warranting the use of Adaptive design (AD) to ensure optimum confinement of the optical modes.

dependence of Γ_m (Γ_{opt}) on the QW thickness is nearly eliminated. At these In compositions, one can move to a thinner QW and benefit from the higher material gain G (as well as modal gain g) without paying a penalty with the optical confinement, as will be seen in the following sections. This is an advantage of the tunable design methodology selected here, where the laser stack is designed to optimize the confinement of the mode. The inter-dependent impact of the In composition, quantum well thickness, choice of cavity thickness as well as the indirect impact of these variables on the emission, bandgap, refractive index, mobility, and laser metrics is shown in **Figure 64**. This design ideology is a part of the AD methodology employed in the following sections to determine the optimum design for the tensile Ge QW SCH laser. Although the detailed

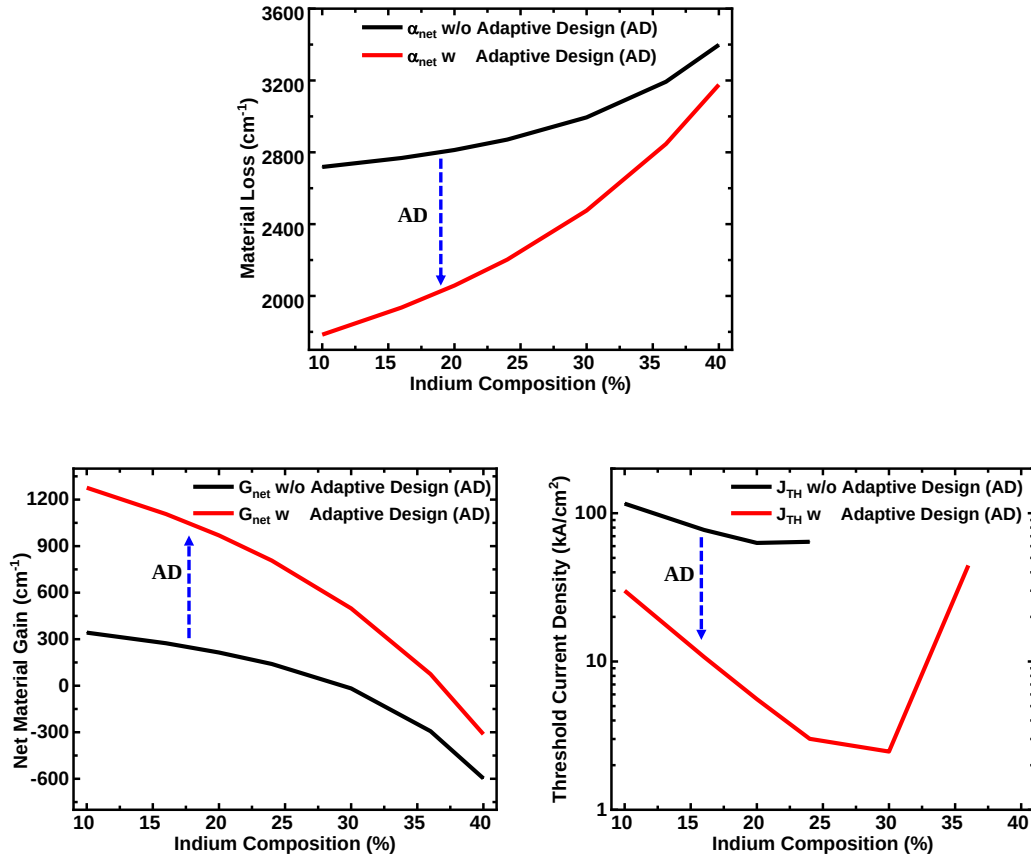


Figure 65. An improvement in three critical laser metrics, loss, net gain and threshold current density due to the AD methodology.

metrics for laser evaluation will be introduced in the following section, the importance of AD on these metrics can be seen here through **Figure 65**. Significant improvement (very critical for

emission from an indirect bandgap laser) in the threshold current density, net gain and loss is seen owing to the design in accordance with AD.

5.8 Tensile Ge QW SCH laser: Max Gain and Gain Spectrum

Utilizing the discussions in the previous sections, the laser metrics such as gain (TE and TM), gain spectrum, net gain and loss can be calculated. The dependence of these on the In composition and quantum well thickness is discussed here. Electrons from the Γ -valley can radiatively recombine with holes from the LH and HH band in the ε -Ge QW. Furthermore, quantization of the bands creates discrete sub-bands in all bands, resulting in radiative transitions from each of them following Fermi's Golden rule [1, 2]. Due to the higher ΔE_c and ΔE_v , at least 1 quantized level can be bound in the ε -Ge finite QW even at room temperature for most of the strain range. These radiative transitions are classified as the ground state transitions (A: $\lambda_{pk(\Gamma1-LH1)}$, B: $\lambda_{pk(\Gamma1-HH1)}$) and the first excited state transitions (C: $\lambda_{pk(\Gamma2-LH2)}$, D: $\lambda_{pk(\Gamma2-HH2)}$). Each of these transitions show distinct lasing gain spectra and threshold performance, shown below, with the ground state transitions being the most dominant transition. The material gain, G (where modal gain, $g = G\Gamma_{opt}$) [3] of the ε -Ge QW is calculated as a function of emitted photon energies. In the ε -Ge/InGaAs QW laser design, the degeneracy between LH and HH bands is broken due to the biaxial tensile strain, and transitions from their corresponding sub-bands would be competing for gain while also resulting in different polarizations (TE or TM) of light. Also, the cavity will support many other modes, and the accurate optical polarization would be quasi-TE or quasi-TM, here the analysis is done for the fundamental mode. In QW structures, this relative transition probability is re-distributed between TE and TM modes unequally, the Γ -LH transition would only contribute to the material gain of the TM mode (G_{TM}) and the Γ -HH transition would contribute largely to the material gain of the TE mode (G_{TE}). The material gain (G) spectrum is computed in the broad range of energy from 0.3 - 1.2 eV to resolve any features associated with at least 4 major peaks (labeled as A, B, C, D), and their movement with increasing tensile strain and QW thickness. The injection of carriers by pumping needed to overcome losses such as, mirror loss of the Fabry-Perot cleaved facets and free carrier absorption (FCA) are quantified through threshold current density (J_{TH}) and carrier density (N_{TH}). The laser-gain solver calculates the net material gain (G_{net}) beyond all material losses, considering three main sources of loss: FCA (α_{fca}), optical confinement loss due to the narrow QW and the mirror loss (α_m) due to the cleaved Fabry-Perot oscillator mirrors. The dominant source of modal loss in a QW is α_m since the small Γ_{opt} scales the α_{fca} making it a lesser concern. Unfortunately, due to the higher emission wavelengths attributed to the high tensile

strains in Ge, the FCA is expected to increase. However, the drastically lower J_{TH}/J_{TR} and N_{TH}/N_{TR} associated with these low band bandgap materials, as well as the low doping will reduce the FCA. Hence, to simplify the analysis, considering the large variation in reported FCA values for ϵ -Ge laser structures, we have assumed a constant and high FCA of 500 cm^{-1} [14] [8, 13, 16, 33]. The proposed ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ QW laser structure can provide considerable net gain even if the FCA is an order of magnitude larger than expected. Note that at the wavelength of operation, the FCA associated with InGaAs waveguide and Q-barrier is expected to be orders of magnitude lower than Ge. Beyond the threshold condition for overcoming all the losses listed above, additional pumping will result in an additional gain which eventually saturates at a value identified as the maximum material gain G_{max} .

With an increase in In composition, the bandgap of $\text{In}_x\text{Ga}_{1-x}\text{As}$ reduces whereas the electron mobility and refractive index increases, impacting the total electrical and optical properties of the QW layer stack. The ground state eigen energies for electrons and holes in the ϵ -Ge QW are determined by the finite band offsets as well as the effective masses and band deformation, all of which are dependent on the tensile strain and consequently the In composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$. The gain spectrum of the ϵ -Ge laser can be significantly tuned by altering the In composition in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide layer. And this variation of the gain spectrum for the TE and TM modes is shown in **Figure 66** for a 10 nm Ge QW, respectively. With an increase in In composition, the tensile strain in Ge increases, the LH-HH band degeneracy breaks, and the LH band moves upward, tending towards dominance. All the peaks are seen to move to lower energies indicating an overall

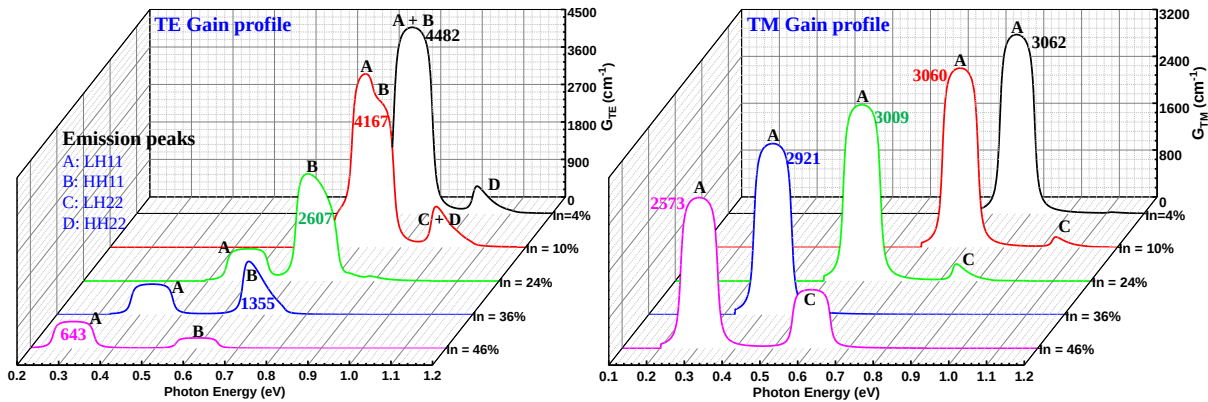


Figure 66. Material gain for the TE (left) and TM (right) modes for the tensile Ge QW laser, for different In compositions. The 4 major peaks associated with key direct transitions are highlighted along with the gain number for the max peaks.

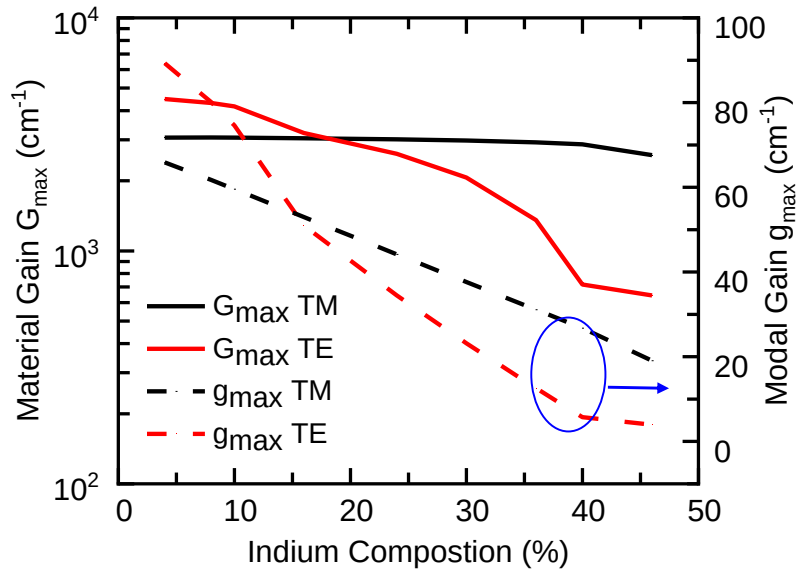


Figure 67. The maximum material gain as well as the modal gain for the TE and TM modes as function of different In compositions and corresponding tensile strain in Ge.

redshift. The quantization effect for the sub-bands is evident. A constant fermi level separation in the QW is maintained for all the configurations above for the different spectra. The adaptative design is used to tune the cavity based on the previous discussion to ensure a maximum

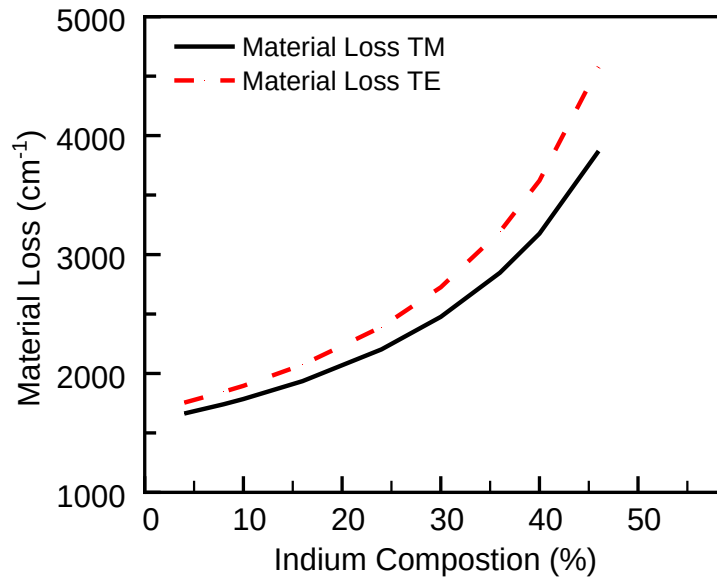


Figure 68. The material losses experienced by the two lasing modes for different In composition. The changing emission wavelength with In composition affects the optical confinement and hence the losses.

confinement factor. The maximum values of the material gain and the modal gain for the TE and TM modes are summarized as a function of In composition in **Figure 67**. The TE gain depends strongly on the HH contributions as seen earlier through the transition matrix element, this causes the TE gain to drop with increasing In composition and can be seen through the TE polarization gain spectrum. The gain coefficient term which accounts for the transition probabilities and the transition matrix element has a drastically different trend for the transitions from LH (nearly constant) and HH (decreasing) bands. The LH band transitions are always aligned with the bandgap of ϵ -Ge resulting in a nearly constant trend, and correspondingly a constant gain profile for the TM mode is obtained.

At the threshold condition beyond transparency, the modal gain g reaches the threshold and is equal to the total losses, i.e., $g = g_{th} = \alpha_{tot}$. Here, $\alpha_{tot} = \alpha_{fca}\Gamma_{opt} + \alpha_m + \alpha_{others}$, is the total loss associated with the ϵ -Ge QW laser structure. The TE mode experiences more material losses compared to the TM mode (see, **Figure 68**) due to the slight difference in the optical confinement factor due to a higher energy of emission attributed to the Γ -HH compared to Γ -LH emission resulting in a higher refractive index of InGaAs. Impact of In composition in the ϵ -Ge/InGaAs single QW (SQW) cavity on the total material losses ($\frac{\alpha_{tot}}{\Gamma_{opt}}$) is shown in **Figure 68**. The

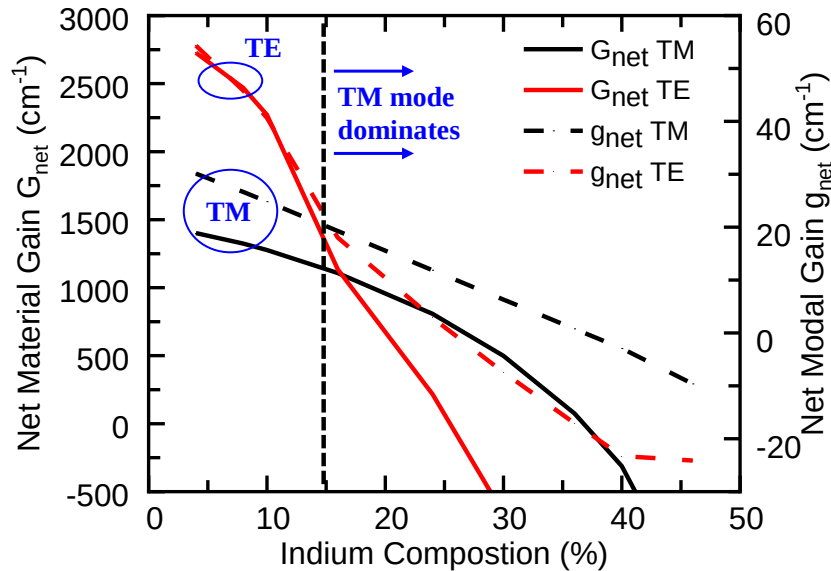


Figure 69. Combining the material gain and material losses to obtain the net material and modal gain available as a function of In composition. The transition point where Ge QW laser moves from a TE polarized laser to a TM polarized laser is identified at In = 15 % corresponding to a tensile strain of ~ 1 %

net material gain and modal gain beyond all losses are shown in **Figure 69**. It is evident that the TM mode dominates at higher In compositions by providing a higher modal gain. The transition point where the Ge QW laser moves from a TE-polarized laser to a TM-polarized laser is identified at In = 15 % corresponding to a tensile strain of ~ 1 %. The impact of the In composition in the underlying InGaAs layer and the corresponding tensile strain in Ge, on the gain spectrum, gain peaks, loss and net material and modal gain has now been discussed. A discussion on the quantum well thickness is next.

Evidently, the Ge QW laser can provide good lasing performance over a wide range of emission wavelengths and In compositions, along with certain challenges and trade-offs. Due to the pseudomorphic growth of Ge on InGaAs, the strain-field creates a certain degree of roughness,

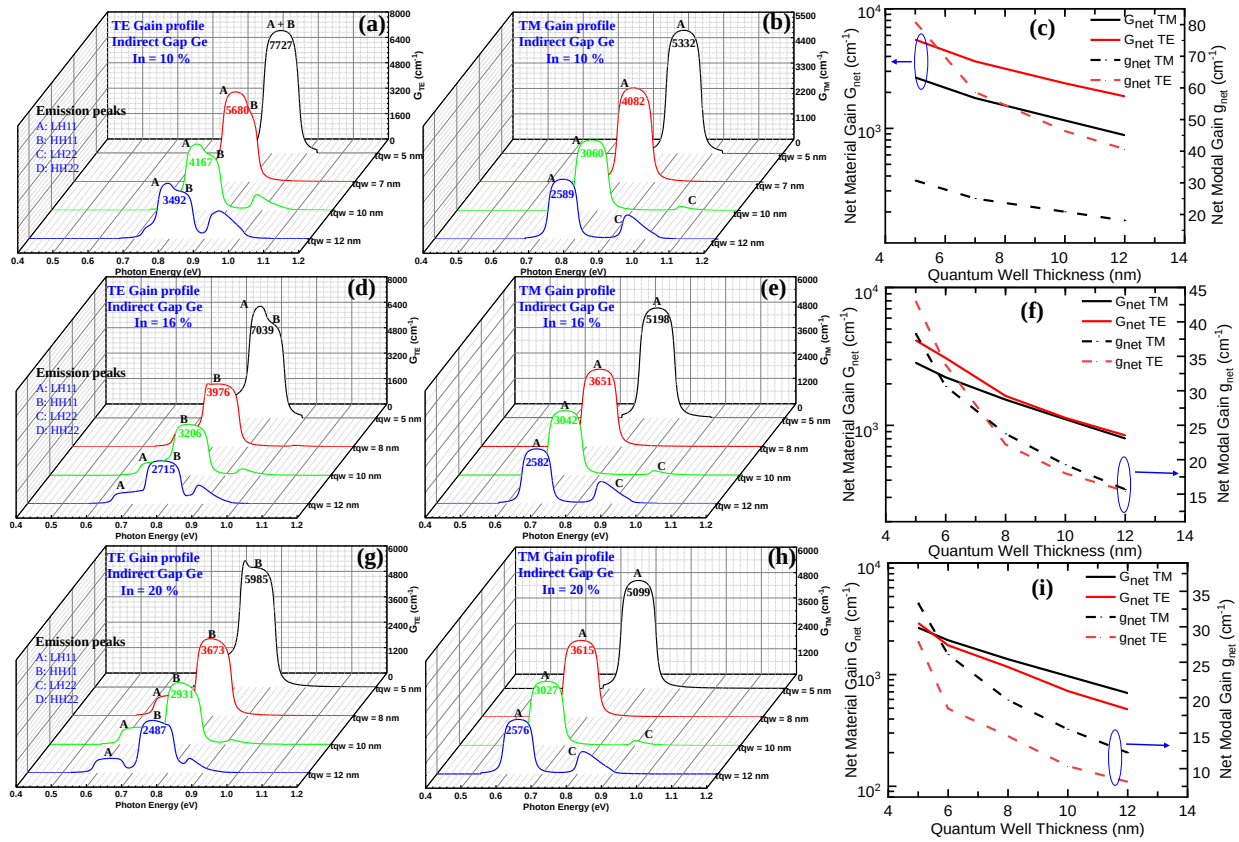


Figure 70. The proposed Ge/InGaAs QW laser with indirect bandgap Ge as a function of QW thickness. Gain spectrum for the (a) TE and (b) TM mode for an In composition of 10 % with IQE ~ 0.5 % and but with very high (c) net gains. Gain spectrum for the (d) TE and (e) TM mode for an In composition of 16 % with IQE ~ 2 % and high (f) net gains. Gain spectrum for the (g) TE and (h) TM mode for an In composition of 20 % with IQE ~ 4 % and high (i) net gains.

interdiffusion, and non-ideality at the interface. Owing to the superior growth quality these non-idealities have been reduced to the lowest possible value of ~ 0.6 nm [30] which indicates an ultra-abrupt interface with the precision of a single monolayer, consequently, this places a lower limit on the thickness of the Ge QW for reliable fabrication and operation. Thus, in this work, we study the QW thicknesses above 5 nm to limit the transition layers to within 20 % of the QW thickness. Further reducing the QW thickness is not expected to significantly affect the modal gain of a conventional QW laser due to the inverse impact of the QW thickness on the DOS (increasing) and optical confinement (decreasing) [34]. Considering the improved IQE for the tensile Ge QW with large In compositions and correspondingly long emission wavelengths, the design ensuring maximum possible confinement factors is crucial. Such a configuration is possible by avoiding very small quantum well thicknesses along with the adaptive waveguide design discussed earlier. The impact of the QW thickness on the gain spectrum for the TE and TM polarization is shown in **Figure 70**, at a fixed bias and low In compositions where Ge QW is still an indirect bandgap material. For In = 10 % in **Figure 70(a-c)**, the Γ -HH transitions are still dominant over the Γ -LH transitions even though the LH band has risen significantly above the HH band as expected from the band deformation due to tensile strain seen earlier in this section. This phenomenon occurs due to two effects: (i) the significantly higher DOS of the HH band and (ii) the much lighter effective mass of holes in the LH band resulting in larger eigen energy and consequently reduced effective difference between the ground state energies of the HH and LH bands. For example, in **Figure 70(a)** at $t_{\text{qw}} = 5$ nm, the LH band ground state energy has risen nearly equal to the HH band ground state energy ($E_{\text{tr}} \sim 0.9$ eV), resulting in an overlap of their respective gain peaks for the TE mode (note that although the peak locations are overlapping the gain contributions will be vastly different due to the different DOS). This observation can be further verified through the G_{TE} peak location for $t_{\text{qw}} = 5$ nm in **Figure 70(b)** which is also at ~ 0.9 eV, confirming that the LH and HH band ground states are nearly at the same energy in this configuration. As the t_{qw} is increased beyond 5 nm, the LH band ground state can be seen to move upwards resulting in distinguishable A: $\lambda_{\text{pk}(\Gamma\text{-LH1})}$ and B: $\lambda_{\text{pk}(\Gamma\text{-HH1})}$ peaks. Higher order excited state peaks C: $\lambda_{\text{pk}(\Gamma\text{2-LH2})}$ and D: $\lambda_{\text{pk}(\Gamma\text{2-HH2})}$ move farther away from the peak emissions as t_{qw} is reduced, and the probability of their excitation as well as the material gain associated with them drops exponentially. For the TM polarization, the contributions to the material gain arise only from the LH transitions thus, only A: $\lambda_{\text{pk}(\Gamma\text{-LH1})}$ and C: $\lambda_{\text{pk}(\Gamma\text{2-L2})}$ are visible in the gain spectrum. As the thickness is increased to 12 nm and beyond, the

quantization effects start to diminish and the higher-order peaks begin to merge creating a broad low-material gain spectrum.

The net material and net modal gain of the TE mode for indirect bandgap Ge at $\text{In} = 10\%$ is summarized in **Figure 70(c)** indicating that the TE mode will dominate the laser performance. Although a very high net modal gain for the TE mode can be achieved in this configuration, the expected IQE is $\sim 0.5\%$ and the J_{TH} is expected to be $\sim 100 \text{ kA/cm}^2$, as will be seen in the next section. As the QW thickness is reduced, the ground state eigen energy in the Γ -valley rises rapidly due to the low effective mass. The carriers can increasingly occupy the indirect L-valley, partially negating the effect of the tensile strain by lowering the transition probability and increasing the quasi-fermi separation required for transparency. At $\text{In} = 16\%$, the net modal and net material gains are nearly equal between the TE and TM modes as the QW thickness is varied, as seen in **Figure 70(d-f)**. Here, the spectrum has shifted to slightly lower energies compared to $\text{In} = 10\%$ in **Figure 70(a) and (b)** owing to the tensile strain. Furthermore, the LH band ground state is always visibly higher than the HH band ground state for all t_{qw} (large LH and HH band separation) resulting in distinct peaks (see, **Figure 70d and e**). The TE gain is contributed primarily from the

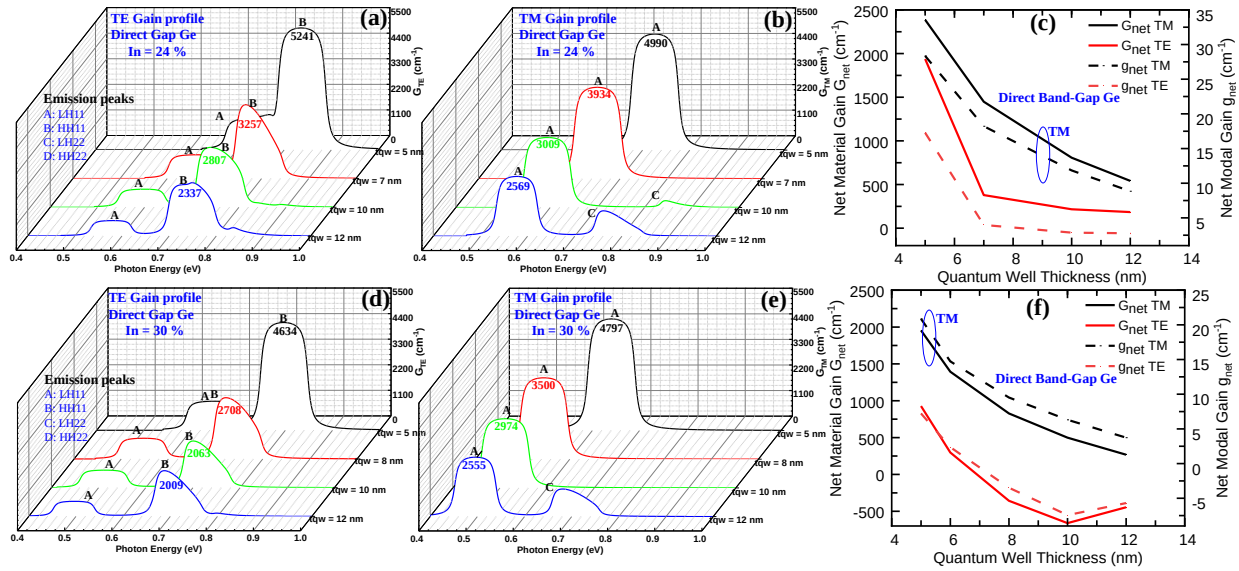


Figure 71. Direct bandgap lasing from the proposed Ge/InGaAs QW laser for various QW thicknesses. Gain spectrum for the (a) TE and (b) TM mode for an In composition of 24 % with IQE $\sim 8\%$ and with moderate (c) net gains. Gain spectrum for the (d) TE and (e) TM mode for an In composition of 30 % with IQE $\sim 20\%$ and acceptable (f) net gains. Beyond $\text{In} \sim 36\%$, the material gains cannot overcome the losses in SQW configuration for the Ge/InGaAs QW laser.

B: $\lambda_{pk(\Gamma_1-HH1)}$ peak owing to the much larger DOS of the HH band. Here, at In = 16 %, the quantization effect, optical confinement, losses, broken degeneracy of LH and HH bands, and higher DOS of HH band, effectively cancel out the differentiating effects of each other resulting in nearly equal net material and net modal gains for the TE and TM polarizations (see, **Figure 70f**). Moving to In = 20 %, the Ge QW is nearly direct bandgap and an IQE of nearly 4% can be achieved in this configuration. Consequently, the TM gain dominates by providing the higher net modal gain, and the gain profiles for the TE and TM modes are shown in **Figure 70(g-i)**. One can note from **Figure 70**, that the modal gain can be increased significantly by reducing the QW thickness owing to the tunable cavity design.

The gain spectra for the TE and TM modes for direct bandgap Ge at In = 24 % and In = 30 % are shown in **Figure 71(a-c)** and **Figure 71(d-f)** respectively. Due to the significant separation between the LH and HH bands, the dominant contributions to the TE and TM mode material gains are from the HH and LH valley respectively. The TM mode provides a higher material gain as well as net modal and net material gain as Ge is a direct bandgap material and LH band emissions are dominant. The In = 20 % SQW near-direct bandgap laser structure proposed in **Figure 71(g-i)** can provide a TM net modal gain of $\sim 20 \text{ cm}^{-1}$ for a reasonable t_{qw} of $\sim 8 \text{ nm}$, at an IQE of 4%. Consequently, at In = 30 % using the direct bandgap Ge the net modal gain of 10 cm^{-1} can be achieved at t_{qw} of $\sim 8 \text{ nm}$ and 20 cm^{-1} at t_{qw} of $\sim 6 \text{ nm}$, with an IQE of 20 %. The net material gain available in these QW structures is large and moving to MQW architectures can drastically scale the net modal gain. Beyond In $\sim 36 \%$, the modal gain cannot overcome the modal loss and the Ge SQW laser cannot lase (migrating to MQW or low-loss cavities is a potential solution).

5.9 Tensile Ge QW SCH laser: Injection, Threshold and IQE

After discussing the gain spectrum, modal gains and net gains that the tensile strained Ge laser can provide and the impact of In composition and quantum well thickness, it is important to quantify the amount of current/carriers required to achieve lasing threshold and maximum gain. Further, it is also crucial to understand the internal quantum efficiency for the particular emission wavelength, which determines the fraction of carriers which participate in radiative transitions and the rest which are lost to heat generation. Here the impact of the In composition and quantum well thickness on the injection characteristics, threshold and IQE is discussed.

At the injection level of threshold current density J_{TH} (correspondingly N_{TH}), the modal gain g reaches the threshold and is equal to the total losses, i.e., $g = g_{th} = \alpha_{tot}$. Here, $\alpha_{tot} = \alpha_{fca}\Gamma_{opt} + \alpha_m + \alpha_{others}$, is the total loss associated with the ϵ -Ge QW laser structure. The maximum material gain G_{max} as a function of injected charge density and total current density is shown in **Figure 72(a) and (b)**, respectively, for In = 4% (indirect bandgap Ge), In = 24 % (direct bandgap Ge) and In = 36 % (strongly direct bandgap Ge). At In = 24, 36 %, the G_{max} shown in **Figure 72(b)** up to injected current levels of ~ 100 kA/cm² is due to the dominant VB, which is

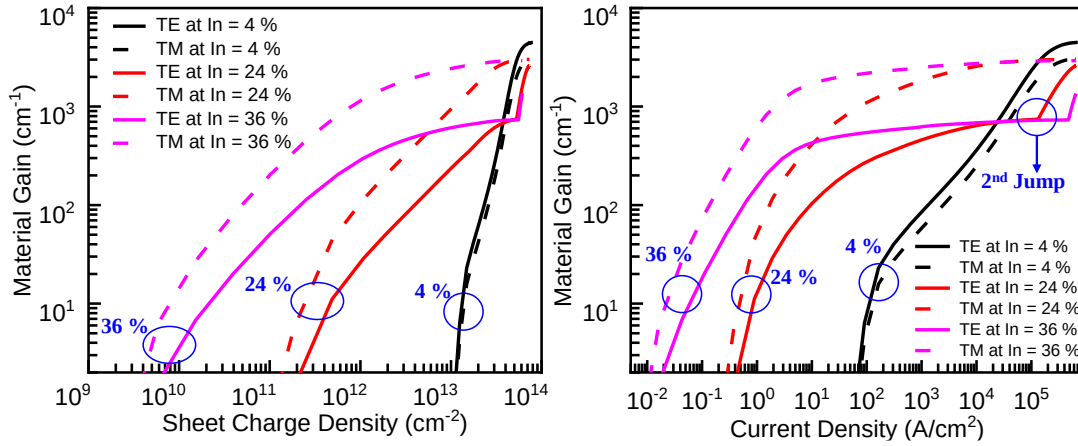


Figure 72. In composition and tensile strain effect: Material gain of the Ge QW laser as a function of injected (left) sheet charge and (right) current density, at In = 4, 24 and 36 % for the TE and TM modes.

the LH band. A second jump in TE gain is observed at very high injection levels due to HH band transitions which are at a significantly larger energy separation than the dominant band-edge, i.e., LH band. The bias dependence of the emission peak for the TE mode is also seen in **Figure 73(b)**.

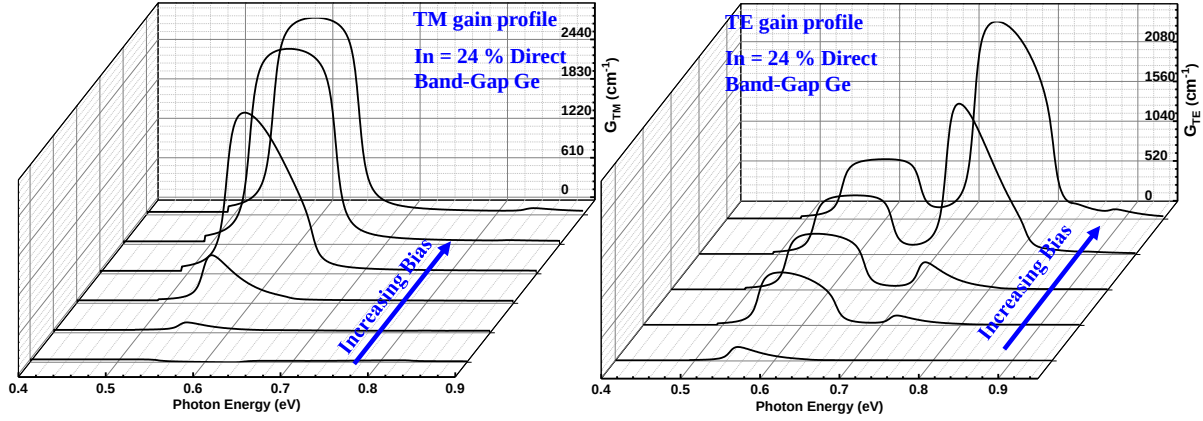


Figure 73. Gradual increase in material gain with increasing current bias as population inversion occurs for direct bandgap Ge at In = 24 % with (a) TM mode and (b) TE mode. The dependence of emission wavelength on the biasing condition is clear for the TE mode.

To reach this second jump of TE gain, the In = 36 % requires a much higher injected current density than the In = 24 % case, as the HH band is further away. Thus, for the TE mode, the peak energy (consequently λ_e) varies drastically with applied bias and injection condition, as the G_{TE} depends on LH and HH sub-band transitions. Such a jump and associated complications will not be possible for the TM mode as only the LH emissions contribute to the TM mode gain, resulting in an operating wavelength that is stable to bias variations.

From **Figure 72(a) and (b)**, it is also evident that the TE and TM modes provide similar gain and injection characteristics for low tensile strain configuration, *i.e.*, In = 4 %. In this case, very high injection densities are needed to reach transparency and consequently lasing threshold. Thus, an unstrained/low-strained Ge QW laser can provide comparable TE and TM gains at sufficiently high injection levels. To achieve lasing at lower injection densities, one must move to higher tensile strain, *i.e.*, higher In composition which results in drastically different performance between the TE and TM modes, with TM mode lasing at lower injection levels and providing higher material gain. As one approaches higher In compositions three observations can be made: (i) low injection lasing is possible only from the TM mode, (ii) G_{TE} reduces drastically whereas G_{TM} remains nearly constant, and (iii) modal gain reduces monotonically due to decreasing Γ_{opt} .

Interestingly, G_{TE} as well as the TE mode peak wavelength is bias dependent, unlike the TM mode (*see, Figure 73 a and b*). At low bias, the LH band which is the dominant VB is excited easily and provides a gain peak. At higher bias (high current pumping), the quasi-fermi level separation is large enough to excite the LH as well as the HH band and a second peak of higher

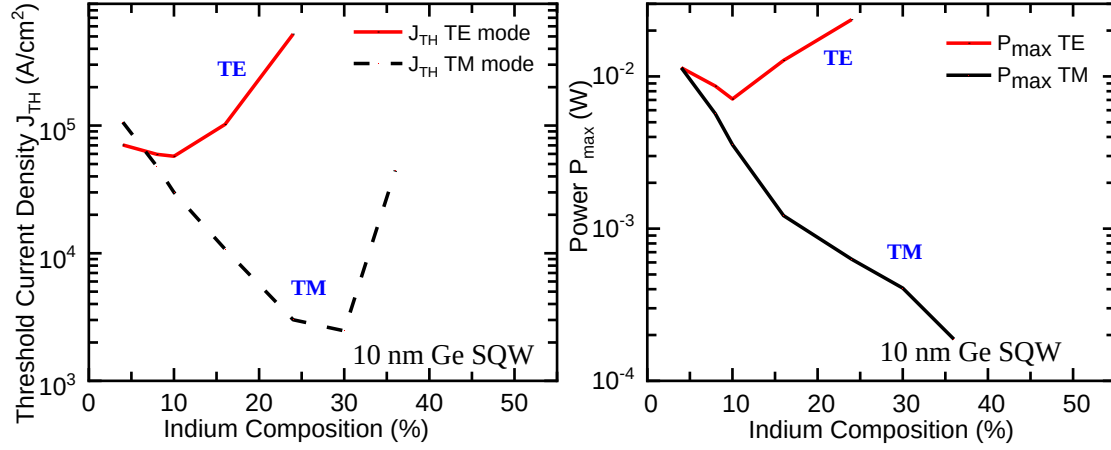


Figure 74. (left) Threshold current density as a function of In composition in the Ge QW laser showing that direct bandgap Ge can provide TM lasing at ~ 2 kA/cm² for a 10 nm QW which is a significant improvement over existing Ge lasers. (right) Total power consumption by the entire SCH QW laser to achieve maximum gain beyond losses as a function of In composition.

DOS, i.e., HH band can be seen. The TE gain is dependent strongly on the HH band emissions, which move to increasingly higher energy separations as the tensile strain in Ge is increased resulting in the need for a significantly higher injection level to achieve lasing. It can also be observed that beyond In ~ 40 %, the LH band transitions provide the TE gain peak as the contributions from the HH band to the TE gain have dropped significantly.

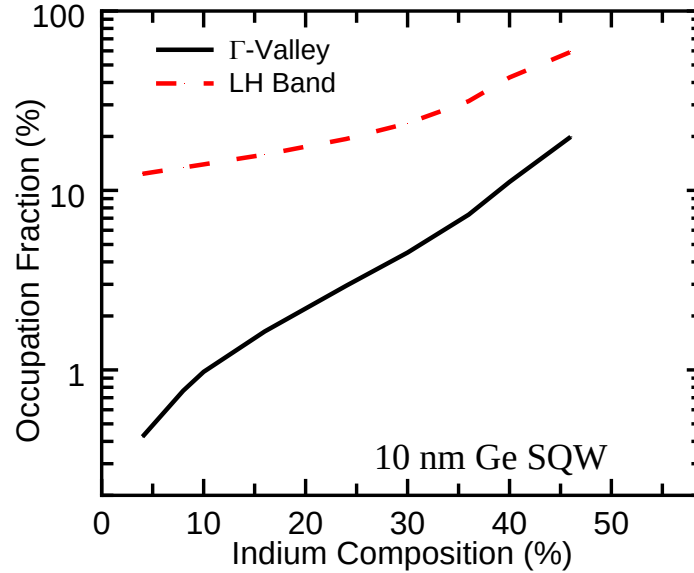


Figure 75. Occupation fraction of the direct bands, i.e., LH valence and Γ conduction band as a function of In composition. The increasing tensile strain improves the occupation of the direct band Γ -valley and LH-band.

The J_{TH} variation with In composition is shown in **Figure 74**. At lower In compositions, the J_{TH} is high due to indirect bandgap Ge as the lasing medium resulting in a very small fraction of carriers occupying the Γ -valley while majority of the carriers occupying the L-valley creating a high transparency current density (see **Figure 72**). The power consumption required to achieve the maximum gain beyond all losses is shown in **Figure 74**. The J_{TH} can be reduced by increasing the tensile strain in Ge and thus increasing the Γ -valley (and LH band) occupation fraction as shown in **Figure 75**, but this also increases the material losses (inverse relation to confinement factor). Thus, the optimum J_{TH} which can be attained considering the two competing mechanisms with increasing In composition: reducing confinement factor and increasing Γ -valley occupation, is ~ 2 kA/cm² at In ~ 30 %. Beyond In ~ 36 %, the material losses are too large to overcome in this cavity configuration, resulting in loss of lasing. The tensile strain in Ge lowers the Γ -valley faster than the L-valley resulting in a gradual increase in carrier populations in the Γ -valley, as seen in **Figure 75**. As the Γ -valley lowers further with increasing In composition, the ε -Ge active layer starts to favor the direct radiative transitions resulting in an improved IQE.

The internal quantum efficiency (IQE or η_i) is the ratio of radiative recombination rate to the total recombination in the ε -Ge QW laser structure at maximum gain, $\eta_i = \frac{J_{rad}}{J_{rad} + J_{non-rad}}$,

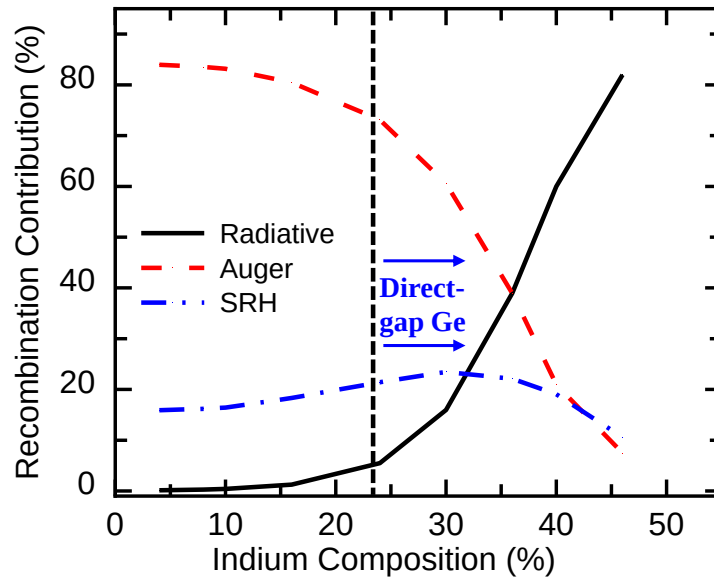


Figure 76. Effect of In composition on relative contributions of different recombination mechanisms as Ge transitions to a direct bandgap material. The superior material quality ensures that the SRH recombination is minimal.

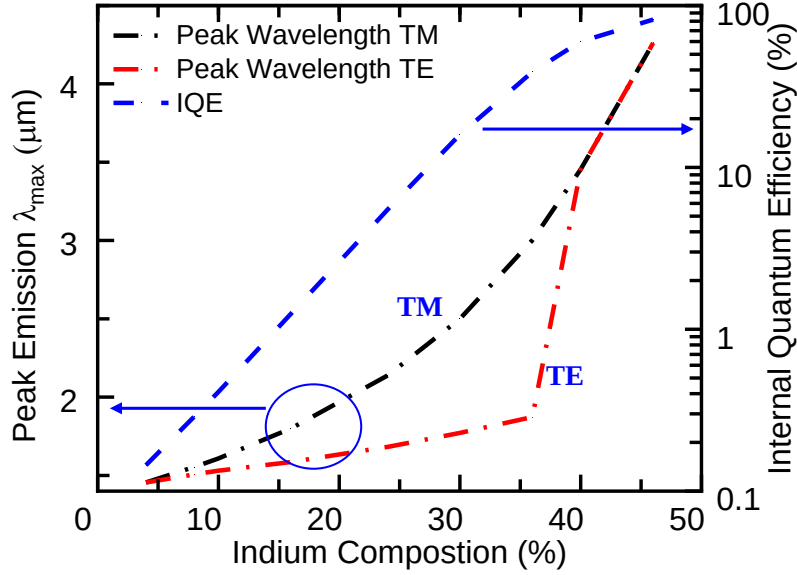


Figure 77. The emission wavelength and IQE as a function of In composition for a 10 nm Ge QW.

where $J_{non-rad}$ includes the non-radiative recombination mechanisms such as SRH and Auger recombination [7], both of which are dependent on the band structure, minority carrier lifetime, and injection density. The IQE quantifies the proportion of the radiative transitions compared to other non-radiative transitions such as SRH and Auger within the Ge active layer. The radiative, SRH, and Auger recombination contributions are dependent on the injection levels, band structure, minority carrier lifetime, doping and intrinsic carrier concentration, see **Figure 76**. The IQE (see,

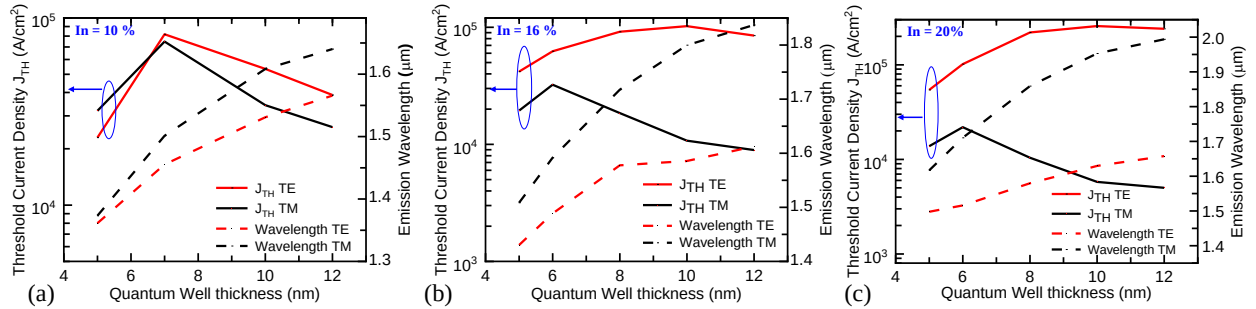


Figure 78. Indirect bandgap Ge/InGaAs QW laser: J_{TH} and emission wavelength as a function of QW thickness, (a) In = 10 %, (b) In = 16 % and (c) In = 20 %.

Figure 77) has improved at higher In composition due to the increase in radiative recombination within the active layer, but this improvement is limited by the Auger recombination which remains an issue for low bandgap materials such as Ge. The In composition (and corresponding tensile strain in Ge) can tune the emission peak over a wide range of wavelengths from 1.55 μm to 4 μm

as seen in **Figure 77**, thus showing potential for a wide range of applications. Beyond $\text{In} = 40\%$, the TE and TM emission peaks for maximum material gain are aligned as this emission is solely from the LH band.

For an ideal cavity of very low material loss, the J_{TH} will increase monotonically as t_{qw} is reduced due to the negative effect of the QW thickness scaling. As the quantum well thickness is reduced, the ground state eigen energies in the VB and CB increase, increasing the effective emission band edge. This results in an increase in emission energy and a consequent decrease in

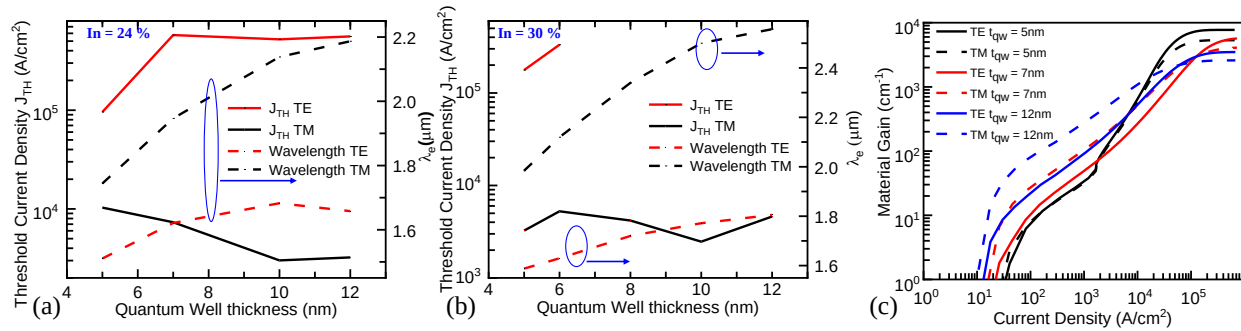


Figure 79. Direct bandgap Ge/InGaAs QW laser: J_{TH} and emission wavelength as a function of quantum well thickness (a) $\text{In} = 24\%$ and (b) $\text{In} = 30\%$. (c) Material gain of the Ge QW laser as a function of injected current density, at $\text{In} = 10\%$.

emission wavelength. The impact of QW thickness on J_{TH} and emission wavelength for the TE and TM polarizations is shown in **Figure 78(a-c)** for indirect bandgap Ge QW laser. At $\text{In} = 16\%$ and beyond, the threshold current density for the TE mode lasing is significantly higher than the TM mode as seen in **Figure 78(b) and (c)**. Although the TE mode provides significant gain as seen earlier, the threshold current required for this gain is significantly higher than the TM mode. Thus, the Ge QW laser can operate with a good net material gain and a decent threshold current density only in the TM polarization. The impact of QW thickness on the J_{TH} and emission wavelength for the TE and TM polarizations is shown in **Figure 79(a-b)** for direct bandgap Ge QW laser at $\text{In} = 24, 36\%$. The threshold current density can be reduced up to 2 kA/cm², at $\text{In} = 30\%$ for the TM polarization with an emission wavelength $\sim 2\ \mu\text{m}$. The impact of t_{qw} scaling cannot be seen directly on the threshold trends in accordance with simple first principle theory, as J_{TH} is a strong function of the loss in the cavity (extracted from the G_{max} v/s J curve) and the specific choice of mirror loss and FCA along with the confinement factor and the current injection characteristics in the 3D structure will cause the trend to differ drastically [10] (see, Fig. **Figure 79c**).

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Chapter 6 –Dielectric spectra for tensile strained Ge thin films

6.1 Overview and motivation for optical characterization of Ge on InGaAs

The previous sections discuss important applications (multi-gate FETs and QW lasers), process benefits, performance improvements, and trade-offs associated with devices made using monolithically integrable Ge thin films which are biaxially tensile strained using InGaAs strain templates. Germanium (Ge) has been gaining popularity for applications in optoelectronics, photonics [1-3], beyond Moore electronics [4-6], and sensing [7], as well as potential applications in quantum technologies [8, 9] over recent years. One common solution for realizing Ge optoelectronics has been integration on a silicon (Si) substrate [10]. However, the growth of Ge on Si has a high lattice misfit ($\sim 4\%$), causing defects and dislocations, hindering optoelectronic functionality through reduced minority carrier lifetime [11,12], and defect-induced shot noise [13]. Furthermore, a coherent light source (an integral component of many on-chip optoelectronic technologies) can be realized monolithically using Ge [10], GeSn [14,15], GeSn/SiGeSn [16], or tensile strained Ge (ϵ -Ge) [1,17] gain media on a Si or GaAs substrate. Additionally, the heterogeneous integration of different monolithic chiplets to form diverse functionalities is an essential step toward scalable quantum technologies [18]. Using monolithically grown Ge-on-InGaAs quantum well (QW) laser chiplet, one may potentially reduce the complexity and cost of the process and enable on-chip optoelectronics. This GaAs-based monolithic configuration (*i.e.*, $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ buffers on a GaAs substrate) is a solution for growing crystalline Ge (apart from the well-controlled tensile strain) for two key reasons: (i) lower defect density due to lattice proximity [1], and (ii) transferability of GaAs technology to Si substrate [1,19]. For the tensile strained Ge on InGaAs (ϵ -Ge/InGaAs) based photonic devices, carrier, and optical confinement are indispensable for efficient operation, and it can be achieved via large band offsets [17] as well as the large differences in the refractive indices [1, 17] between the waveguide and cladding semiconductors. The band offsets as a function of strain in Ge layers grown on $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffers were determined using x-ray photoelectron spectroscopy, and the dependence of Ge-on-InGaAs band offsets on tensile strain was discussed in Chapter 5 and Ref. 17. The refractive index, dielectric constants, optical properties, CPs, and spin-orbit (SO) couplings as a function of

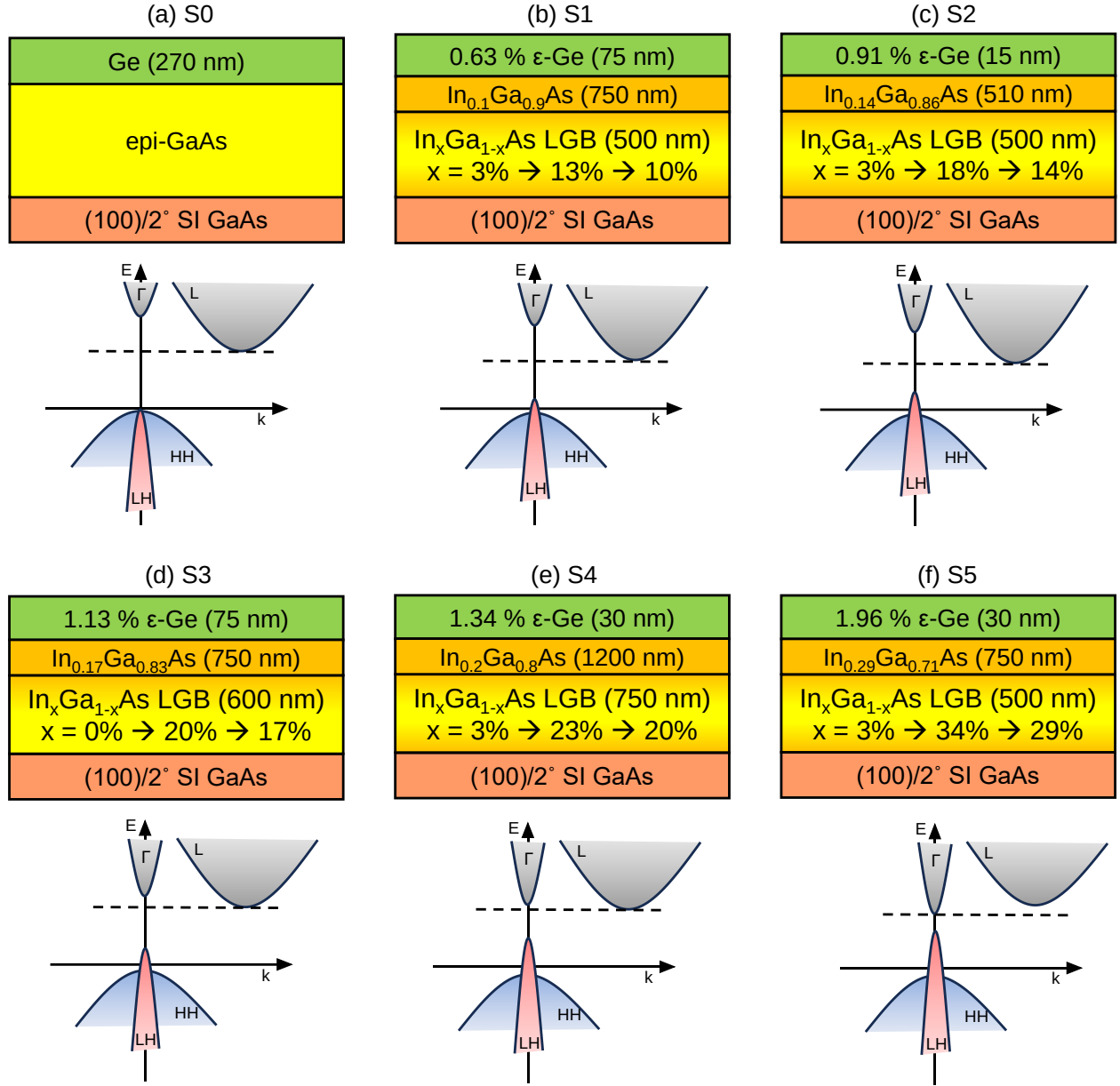


Figure 80. Epitaxial Ge-on-InGaAs structures are grown using MBE and used in this study for optical characterization using VASE. The structures and their corresponding band diagrams are shown in the increasing order of tensile strain (a)-(f) corresponding to S0-S5 from Table I. The tensile strain is achieved using an InGaAs composition-controlled strain template grown on top of a precisely designed linearly graded buffer. These structures also represent the multilayer model used for modeling the VASE data to extract the optical constants.

strain in Ge layer was not demonstrated to date. In the past, the optical properties such as the refractive index ($n + ik$), dielectric functions ($\epsilon_1 + i\epsilon_2$), band structure, absorption coefficient (α),

and Van-Hove singularities (critical points) of unstrained Ge have been studied as a function of growth, measurement temperature, doping, Sn composition, and different growth methods [20-25]. In addition, the impact of biaxial strain on the dielectric constants of Si epi-layers has been studied [26]. However, biaxially tensile strained Ge's optical properties, dielectric constants, and CP transitions were not investigated.

In this section, we explore the impact of tensile strain on the dielectric constants and optical properties of Ge and ϵ -Ge through variable angle spectroscopic ellipsometry (VASE) as a function of tensile strain (ϵ) in Ge via $\text{In}_x\text{Ga}_{1-x}\text{As}$ strain template underneath the Ge layer. The indium (In) composition in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ layer is varied from 0- 29%, corresponding to 0-1.96% tensile strain in Ge. This study aims to highlight the optical properties of epitaxial Ge layers and their dependence on the tensile strain, as the tensile strain is gradually increased between the 6 samples, studied in this work without inducing relaxation-induced defects (*i.e.*, adhering to the critical layer thickness) and maintaining crystallinity [1, 27]. Each sample and their **k.p** calculated band structure [1] schematics are summarized in **Figure 80(a)-(f)** in increasing order of tensile strain in the epitaxial Ge. Similar to the discussion in Chapter 5, the tensile strain moves the Γ -valley downward faster than the L-valley, while also breaking the degeneracy between the LH and HH bands resulting in an upward movement of the LH band. The methodology for the pseudomorphic sample growth is discussed followed by the measurement setup for the VASE system. The model and its goodness of fit are evaluated, and dielectric constants are extracted. A clear shift in the band edge is seen through the absorption spectrum with increasing tensile strain along with an increase in absorption coefficient. Moreover, the direct and indirect bandgap of ϵ -Ge determined from this study is in good agreement with the 30×30 **k.p** calculated results [1]. The Van-Hove singularities in the band structure of ϵ -Ge are discussed and a gradual decrease in the E_0 , $E_0 + \Delta_0$, E_1 , $E_1 + \Delta_1$, and E_0' CPs is seen. Interestingly, it is observed that the SO coupling energy at the Γ -point Δ_0 has a decreasing trend with tensile strain. Whereas the SO coupling energy, Δ_1 in the Λ -direction associated with the E_1 peak remains nearly constant with applied tensile strain. By elucidating the biaxial tensile strain dependence on the dielectric constants of epitaxial thin film Ge, this study opens up an opportunity to improve the design process and analysis of various optoelectronic devices such as ϵ -Ge QW lasers [1, 4, 28], hole-centric spin qubit [29], FinFETs and MOSFETs [4], lattice-matched and unstrained Ge-based nanosheet-FETs [5], photodetectors [30], and photovoltaics [31].

6.2 Optical properties of semiconducting materials

Optical transitions and the link with the band structure of materials, as well as the transitions rates were discussed in Chapter 5. Absorption spectra for materials can be measured using various experimental techniques such as ellipsometry. A fundamental description of the absorption spectrum and optical transition physics is provided here. The readers are advised to refer the preliminary discussion in Chapter 5 along with this section. The absorption coefficient of materials $\alpha(\hbar\omega)$ can be defined as,

$$\text{Abs Coeff} \rightarrow \alpha(\hbar\omega) = \frac{\# \text{ photons absorption rate per unit volume}}{\# \text{ photon injection rate per unit area}} \quad (6.2.1).$$

Thus, justifying the units of (1/cm) for $\alpha(\hbar\omega)$. The term in the denominator is the intensity of optical power incident on the surface of the material per unit energy of the photon $\hbar\omega$,

$$\alpha(\hbar\omega) = \frac{\text{Rate}}{P/\hbar\omega} \quad \text{with} \quad P = \frac{n_r c \varepsilon_0 \omega^2 A_0^2}{2} \quad (6.2.2).$$

The power P has units of W/cm². The net absorption transition rate can be quantified as seen in Eq. 5.1.7 and 5.1.11, just by changing the sign,

$$R_{abs} = \frac{2}{V} \sum_{k_a} \sum_{k_b} \frac{2\pi}{\hbar} |H'_{ba}|^2 \delta(E_2 - E_1 - \hbar\omega) \cdot (f_a - f_b) \quad (6.2.3).$$

The absorption coefficient can thus be calculated as,

$$\alpha(\hbar\omega) = \frac{2}{V} C_0 \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \delta(E_2 - E_1 - \hbar\omega) (f_1 - f_2) \quad (6.2.4),$$

Where the term C_0 is,

$$C_0 = \frac{\pi e^2}{n_r c \varepsilon_0 m_0^2 \omega} \quad (6.2.5).$$

It is crucial to note that the absorption coefficient is independent of the intensity amplitude of the EM wave, A_0^2 . The $\delta(E_2 - E_1 - \hbar\omega)$ can be written as a Lorentzian function to account for line-shape broadening effects. Normalization of the Lorentzian function needs to be taken care of,

$$\int_{-\infty}^{+\infty} L(E_2 - E_1 - \hbar\omega) d\omega = 1 \quad (6.2.6).$$

Note that the broadening mechanism modeled through the Lorentzian function $L(E_2 - E_1 - \hbar\omega)$ was seen earlier in the laser gain calculation in Eq. 5.3.4. The absorption coefficient is related to the dielectric function through the following expression for the imaginary part,

$$\alpha(\omega) = 2 \operatorname{Im} \left\{ \frac{\omega}{c} n_r \left(1 + i \frac{\varepsilon_2}{2\varepsilon_1} \right) \right\} \quad (6.2.7),$$

this can be reduced to obtain,

$$\varepsilon_2(\omega) = \frac{n_r c \varepsilon_0}{\omega} \alpha(\omega) \quad (6.2.8).$$

Combining Eq. 6.2.8, 6.2.6 and 6.2.4, the expression for the $\varepsilon_2(\omega)$ dielectric function can be determined as function of the semiconductor band structure, matrix elements and wavefunctions, as described here,

$$\varepsilon_2(\omega) = \frac{\pi e^2}{m_0^2 \omega^2} \frac{2}{V} \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \delta(E_2 - E_1 - \hbar\omega) (f_1 - f_2) \quad (6.2.9).$$

Further, using the **Kramers-Kronig consistency**, the real part of the dielectric function can also be determined,

$$\varepsilon_1(\omega) = \varepsilon_0 + \frac{2 e^2 \hbar^2}{m_0^2} \frac{2}{V} \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \delta(E_2 - E_1 - \hbar\omega) (f_1 - f_2) \quad (6.2.10)$$

In later sections in this work, the sharp features in $\varepsilon_2(\omega)$ and $\varepsilon_1(\omega)$ will be assigned physical significance and used to interpret changes in the band structure due to biaxial tensile strain. Noting that real measurements have these transitions broadened, the Eq 6.2.9 and 6.2.10 should be modified to include a Lorentzian broadening,

$$\varepsilon_2(\omega) = \frac{\pi e^2}{m_0^2 \omega^2} \frac{2}{V} \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \frac{1}{(E_2 - E_1)((E_2 - E_1)^2 - (\hbar\omega)^2)} (f_1 - f_2) \quad (6.2.11),$$

$$\varepsilon_1(\omega) = \varepsilon_0 + \frac{2 e^2 \hbar^2}{m_0^2} \frac{2}{V} \sum_{k_1} \sum_{k_2} |\langle \vec{e} | p \rangle|^2 \frac{1}{(E_2 - E_1)((E_2 - E_1)^2 - (\hbar\omega)^2)} (f_1 - f_2) \quad (6.2.12).$$

After establishing a relation between the dielectric function and the band structure optical transitions, in following sections we proceed to measurements, modeling and fitting of the VASE data for tensile strained Ge samples.

6.3 Tensile strained Ge-on-InGaAs samples and growth

III-V compound semiconductor templates such as InAlAs and InGaAs that leverage metamorphic and pseudomorphic growth are of interest as they can be used to produce high-quality tunable epitaxial layers for applications in monolithic optoelectronics [1]. As a part of this study, unintentionally (*uid*) doped epitaxial Ge thin films are grown on semi-insulating GaAs (001) substrates. Pseudomorphic ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ structures were realized using a vacuum inter-connected dual chamber solid source molecular beam epitaxy (MBE) system [1, 19, 32]. An isolation between the III-V and the group IV chambers is employed to eliminate atomic interdiffusion at the Ge/InGaAs interface providing an abrupt transition from InGaAs to Ge. The desired In composition in the $\text{In}_x\text{Ga}_{1-x}\text{As}$ strain template was realized using a linearly graded buffer (LGB) grown on a GaAs substrate. This growth process enables a virtually defect-free $\text{In}_x\text{Ga}_{1-x}\text{As}$

Table IV: Summary of ϵ -Ge samples used in this study as a function of In composition. The corresponding changes in the linearly graded buffer (LGB) and the direct bandgap of Ge are highlighted.

Sample Name	In composition (%) in InGaAs strain template	Thickness (nm)			Strain (%) in Ge	$E_{g,\Gamma-LH}$ (eV) λ_g (nm)
		ϵ -Ge	InGaAs strain template	InGaAs LGB		
S0	0	270	0	0	-0.08	0.79 1570
S1	10	75	750	500	0.63	0.675 1837
S2	14	15	510	500	0.91	0.607 2042
S3	17	75	750	600	1.129	0.593 2091
S4	20	30	1200*	750	1.339	0.55 2254
S5	29	30	750	500	1.962	0.42 2915

metamorphic strain template, by restricting defects within the underlying strain-relaxed LGB. In addition, the virtually defect-free pseudomorphic growth of ϵ -Ge on $\text{In}_x\text{Ga}_{1-x}\text{As}$ is possible if the

thickness of the ϵ -Ge layer is maintained lower than the critical thickness of Ge [1, 27]. **Figure 80** and **Table IV** summarize the various ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ structures grown using this MBE system and analyzed to determine the optical properties of ϵ -Ge as a function of tensile strain. Direct bandgaps of ϵ -Ge with varying tensile strain shown in **Table IV** are calculated using the 30×30 $\mathbf{k} \cdot \mathbf{p}$ method [1], and a schematic representation of the relative movement of the band energies of the 4-bands at the Γ -point LH, HH, L and Γ is shown in **Figure 80**. As the thickness of the ϵ -Ge layer is designed to be thinner than the critical layer thickness, the strain is not relaxed and hence the lattice misfit is translated to biaxial tensile strain. Interface abruptness is a critical attribute of determining the quality of the ϵ -Ge/ $\text{In}_x\text{Ga}_{1-x}\text{As}$ heterointerface and a 6 Å heterointerface abruptness was demonstrated for a ϵ -Ge/ $\text{In}_{0.24}\text{Ga}_{0.76}\text{As}$ structure [32] by atom probe tomography using this MBE system and similar growth recipes calibrated using x-ray diffraction and transmission electron microscopy analysis [1, 32-34].

Semi-insulating (100) GaAs wafers that are 2° offcut towards [110] directions were used for this work. Native oxides from the surface of GaAs wafers were desorbed under the presence of arsenic (As_2) overpressure of $\sim 10^{-5}$ torr at 750°C inside the III-V MBE chamber. *In-situ* reflection high-energy electron diffraction was used to monitor surface reconstruction and all stages of the growth of GaAs and InGaAs layers. After the 0.25 μm GaAs layer growth at 650°C , the growth temperature was reduced to 550°C for linearly graded InGaAs buffer and constant composition InGaAs strain template. In each InGaAs graded buffer, inverse grading was incorporated which facilitated the efficient strain relaxation process [35]. Following the InGaAs buffer growth, each sample was cooled down below 175°C and then vacuum transferred to the group-IV growth chamber for Ge epitaxy. A growth temperature of 400°C (thermocouple temperature) and a growth rate of ~ 0.07 Å/s, were maintained throughout the Ge layer growth. More details of the growth procedure and material analysis for this MBE-grown tensile strain Ge on the InGaAs system can be found elsewhere [1, 17, 32-34].

6.4 VASE Measurement methodology and modeling

Samples with varying In composition (S0-S5, *see Figure 80 and Table IV*) were mounted each onto the vertical stage of the J. A. Woollam variable-angle-of-incidence ellipsometer system [36]. The collection of data was performed for all the samples in the range of 0.5 eV to 4.1 eV at room temperature and on the same day to avoid discrepancies due to changes in ambient and equipment configuration. The data was acquired over 4 angles of incidence for all the samples namely 60°, 65°, 70°, and 75° chosen to be around the approximate Brewster's angle for Ge. A broadband Xenon lamp served as the light source, followed by a monochromator for wavelength selection. The incident light was polarized, and its polarization state was altered upon reflection from the sample surface. The reflected polarization was analyzed using a rotating analyzer and detected by a thermoelectrically cooled silicon/strained InGaAs stack photodiode detector. This process determined the ellipsometric angles ψ (amplitude ratio) and Δ (phase difference). The VASE measurement yielded ψ and Δ values with error bars of approximately $\pm 0.02^\circ$ and $\pm 0.06^\circ$, respectively, for each sample studied here. These two quantities, ψ , and Δ , are related to the p- and s-polarization intensities through the relation [36, 37]:

$$\rho = \frac{R_p}{R_s} = \tan(\psi) e^{i\Delta} \quad (6.4.1)$$

where, ρ is the reflection coefficient ratio, R_p and R_s are the Fresnel Reflection coefficients [36, 37]. The p-polarization is defined parallel to the incident plane and the s-polarization is perpendicular, thus forming an orthogonal coordinate system. For a single-layer structure like a smooth surface bulk substrate, ψ and Δ values can be directly converted to extract the refractive index (n) and extinction coefficient (k). However, for the multilayer structures studied here (*see Figure 80*), direct extraction of the optical constants from raw data is not feasible. This is because ψ and Δ are coupled indicators of the optical properties of all the layers, including the surface conditions. An iterative process is necessary to decouple the contributions of each layer in the stack (*see, Figure 80*) and determine their corresponding wavelength-dependent dielectric constants and thicknesses.

The objective of forming an accurate model is to decouple and extract the optical properties of Ge (n , k , ϵ_1 , ϵ_2 , and α) as a function of tensile strain from the measured values of ψ and Δ . The optical constants of InAs, GaAs, and $\text{In}_x\text{Ga}_{1-x}\text{As}$ are known as a function of wavelength and are available with the proprietary software suite WVASE provided with the J.A. Woollam VASE equipment [36]. The individual layer thicknesses and compositions of all the layers in the stack are known through precisely controlled MBE growth recipes calibrated with TEM and x-ray diffraction measurements [1, 32-34] over the years. Due to the correlated nature of the optical constants and layer thicknesses, the thicknesses are held nearly constant around their nominal values during the regression analysis. This ensured that each best-fit thickness remained close to the global minimum of the mean squared error (MSE). The surface roughness and native oxide were effectively modeled as a single surface layer with its thickness as a free parameter. The index of this thin layer was approximated using the effective medium approximation (EMA) to mix the indices of the Ge film and air in a 50:50 ratio [36, 37]. This EMA layer is present above the Ge epitaxial layer in the model and is not shown in the schematic illustration in **Figure 80**. Furthermore, the LGB shown in **Figure 80** is subdivided into 2 sections representing the In composition gradient in $\text{In}_x\text{Ga}_{1-x}\text{As}$ and the overshoot In composition. The composition-dependent optical constants of $\text{In}_x\text{Ga}_{1-x}\text{As}$ were modeled using a pre-determined composition file that

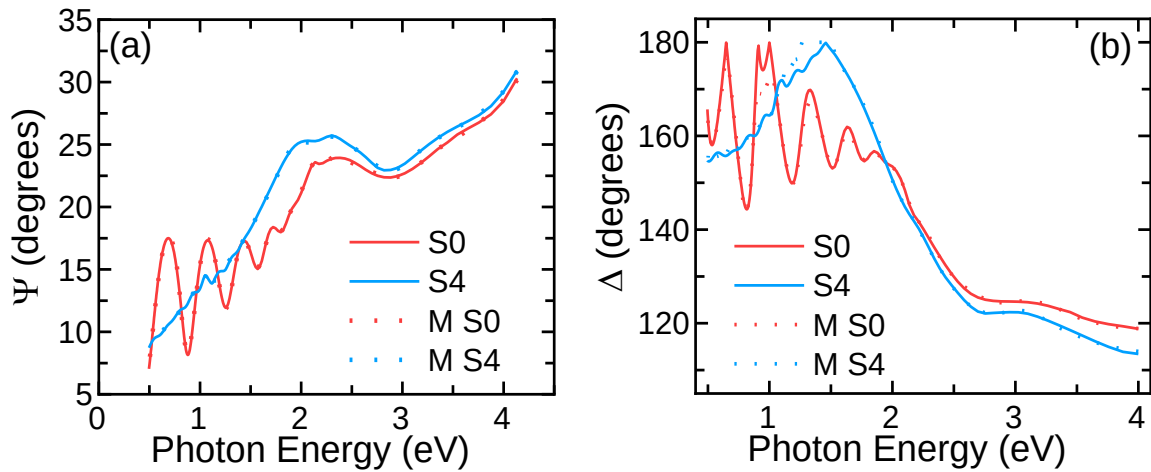


Figure 81. Evaluating the goodness of fit of the model: Measured VASE data and model fit for the extracted (a) ψ , (b) Δ . (c) The corresponding mismatch between the model and measurement calculated as the MSE indicating a good overall fit for all the samples.

significantly minimized the number of fitting parameters. The thicknesses of the LGB sub-sections far away from the top surface are left as free parameters to account for unknown deviations in the optical properties of the LGB due to a high density of mismatch-induced defects. In all cases, this assumption resulted in low MSE by accurately fitting the complex interference oscillations in the ellipsometry data, which arise from the complex multilayer structure beneath the Ge film.

The optical constants for the epitaxial Ge layer were modeled using a Kramers-Kronig consistent General Oscillator (GenOsc) model. The GenOsc layer incorporates multiple parametric *Psemi* oscillators [38] corresponding to various regions of electronic transitions within the band structure measured in the spectra range of 0.5 eV to 4.1 eV. The best-fit result closely matched the optical constants of the reference Ge material [21, 22, 24], *i.e.*, $(\epsilon_1 + i\epsilon_2)$. The optical constants (n and k) of the ϵ -Ge films were determined through a three-step fitting process to mitigate parameter correlations. First, the film thickness and refractive index were uniquely defined using a Cauchy function in the transparent region. Then, with the thickness fixed, the entire wavelength range was fitted to extract both n and k using a point-by-point fit approach [38]. This extended the analysis into the absorbing region (above the bandgap energy). The point-by-point fit provided a good initial estimate, although it didn't strictly enforce Kramers-Kronig's consistency. Finally, a Kramers-Kronig consistent GenOsc model, employing parametric *Psemi* oscillators, was used to refine the optical constants. These oscillators were optimized to match the point-by-point fit results

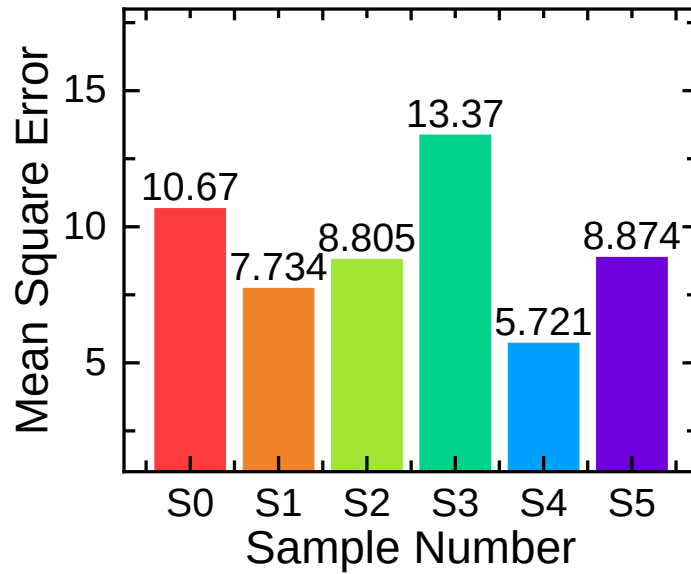


Figure 82. The corresponding mismatch between the model and measurement calculated as the MSE indicating a good overall fit for all the samples.

and then minimize the MSE between the model and the measured spectroscopic data (ψ and Δ). This approach effectively captured the sharp features of the optical constants near the CPs and bandgap energy of the crystalline films. For illustrative purposes, the measured data ψ and Δ , along with the modeled values as a function of photon energy for low and high tensile strained Ge samples are shown in **Figure 81(a) and (b)**, respectively, for one representative angle 70° . A similar method was implemented for all other tensile Ge samples. One can find that there is an excellent agreement between the measured data and the multilayer model for all 6 samples, as evidenced by the low MSE, shown in **Figure 82**.

6.5 Optical constants of tensile strained Ge

After inverting the ψ and Δ values for the multilayer stack model measured and modeled at different angles for the samples over the entire spectrum, the dielectric constants ϵ_1 and ϵ_2 are extracted and shown in **Figure 83(a,c) and (b,d)**, respectively. A clear effect of the tensile strain can be seen on both ϵ_1 and ϵ_2 indicating that there is a shift and/or modulation of the band structure resulting in a change in the CPs. To decode the impact on the CPs, second-order derivatives are extracted and presented in the following sections. A detailed theoretical analysis of the CP trends due to tensile strain is presented. Prior to moving to predictions about other optical constants, CPs and band structures, the extracted dielectric constants from the VASE measurement and models for the unstrained Ge sample S0 can be compared with measurement reports over the years in literature. A comparison of the dielectric constant with literature reports shows a good match, as seen in **Figure 84**.

The refractive index, n and the extinction coefficient, k are shown in **Figure 82** as a function of photon energy as well as the corresponding wavelength. The peak value of n in this energy range can be associated with the critical point $E_1 \sim 2$ eV, which decreases with applied tensile strain while moving from a single peak for unstrained Ge to a double peak for highly tensile strained Ge. These two peaks are associated with the E_1 and $E_1 + \Delta_1$ CPs and can also be seen in **Figure 83** in the form of peaks in the dielectric constants ϵ_1 and ϵ_2 . Increasing the tensile strain results in a reduction in the refractive index at E_1 and $E_1 + \Delta_1$ peaks as well as the movement of the peaks to lower energies. Sample S5 which has the highest tensile strain and is expected to have a strongly direct- bandgap nature is seen to be an outlier to this trend. This may be potentially attributed to the strong deformation of other bands in the BZ, quantization effect associated with the low effective masses of the light hole (LH) and Γ -valley of this highly tensile strained sample (see **Figure 80** and **Table I**) resulting in an increased effective bandgap, or some other phenomenon. The exact cause of this trend is unclear at the time of this study.

In the UV region near 3 eV increasing tensile strain results in a reducing refractive index. The refractive index near the band edge associated with the near-infrared (NIR) region is a cumulative function of the local joint density of states (JDOS), and transitions between direct valleys LH, heavy hole (HH), and Γ as well as the indirect valley L all of which are affected by

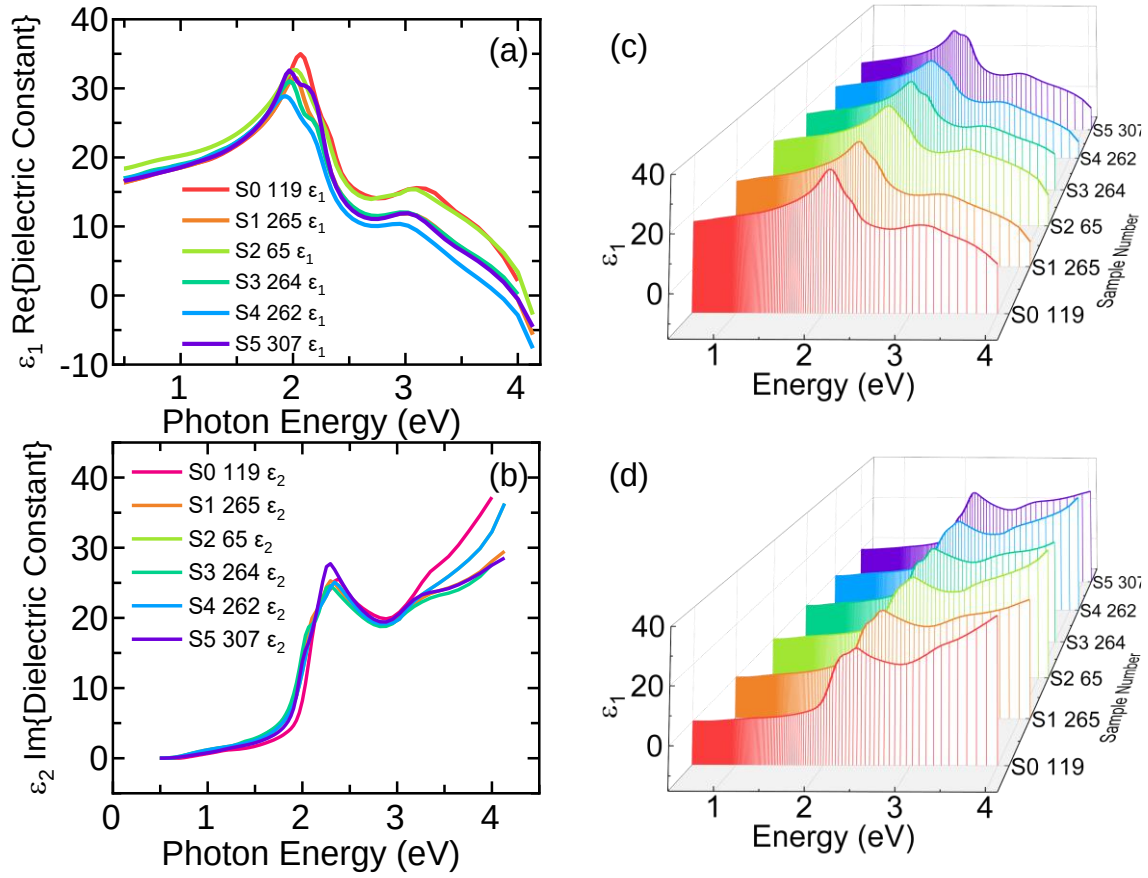


Figure 83. The extracted dielectric constants from the ellipsometric analysis, (a) ϵ_1 and (b) ϵ_2 as a function of photon energy. A 3D contour to visualize the movement of the various CP-related peaks in the dielectric spectrum (c) ϵ_1 and (d) ϵ_2 as a function of photon energy due to epitaxial tensile strain.

the tensile strain. Similar trends can be seen for the extinction coefficient k shown in **Figure 82**. Using the optical spectrum determined for ϵ -Ge, certain interesting trends for the refractive index can be defined in the three regions of particular interest based on the application space, *i.e.*, i) 400 nm UV for photonic and quantum applications, ii) 2 eV region where the E_1 CP peak refractive index lies, and iii) at the band edge of ϵ -Ge for NIR optoelectronics such as Ge QW lasers. The refractive index in these 3 regions is summarized in **Figure 83**. Thus, the optical properties of Ge can be tuned using epitaxial tensile strain during growth via In composition-controlled InGaAs strain template.

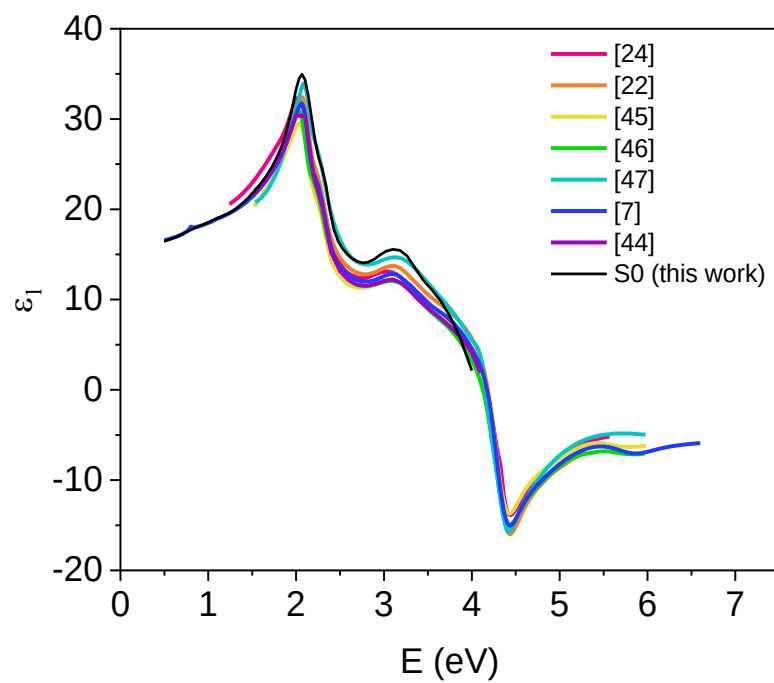


Figure 84. Comparison of the extracted dielectric constant in this work with the unstrained epitaxial Ge sample S0 with existing reports in literature.

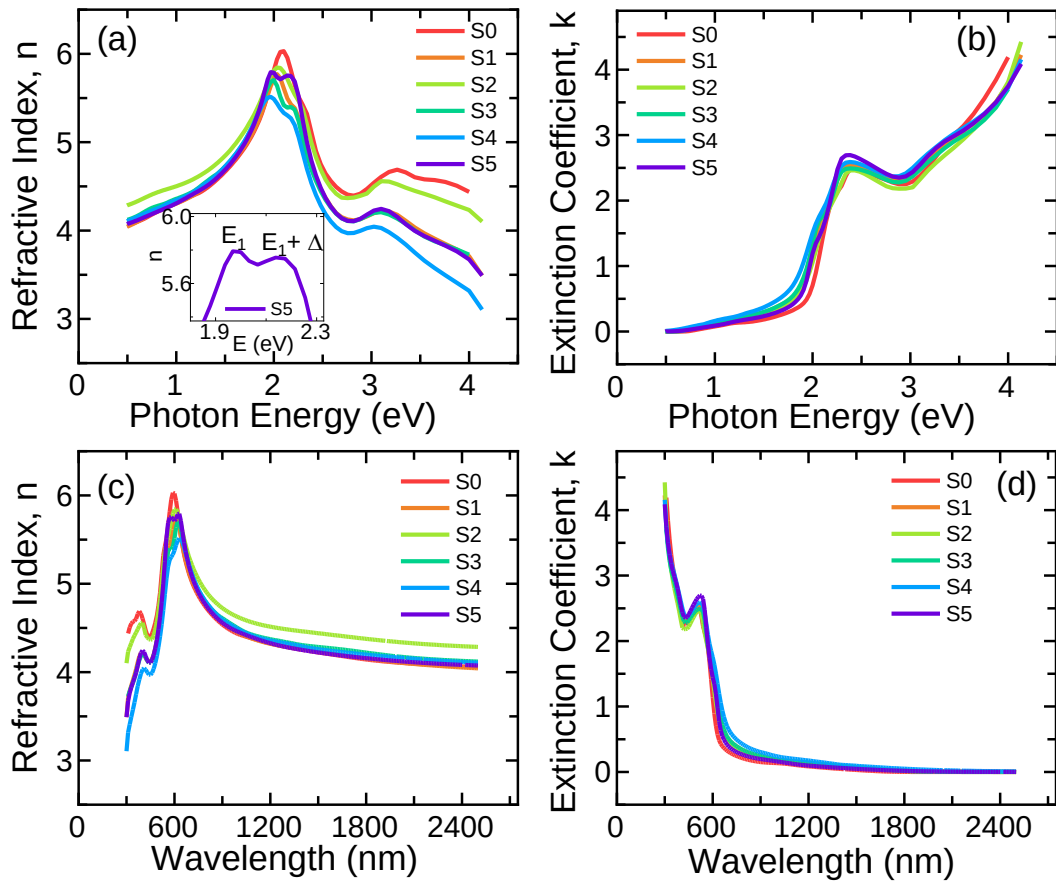


Figure 82. A plot of (a) refractive index n and (b) extinction coefficient k as a function of photon energy for the samples S0-S5 indicating the impact of increasing tensile strain on the optical constants. The optical constants and the impact of tensile strain on a wavelength scale for (c) n and (d) k .

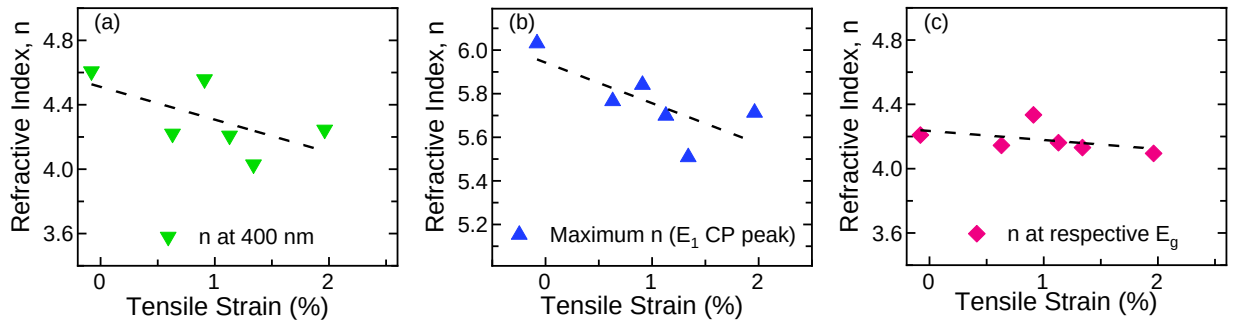


Figure 83. Specific refractive index values as a function of tensile strain, (a) at 400 nm UV region, (b) maximum possible value at the E_1 CP peak, and (c) exactly at the respective $k.p$ bandgaps of each sample S0-S5.

6.6 Absorption spectrum and Tauc band edge movement for tensile Ge

The knowledge of the absorption spectrum for epitaxial Ge and ϵ -Ge can assist in designing and optimizing new light sources such as lasers, LEDs, photodetectors and optical components. The absorption coefficient for the samples S0-S5 in log and linear scale is shown in **Figure 84(a) and (b)**, respectively. As the tensile strain is increased, the bandgap of Ge reduces and an upward shift in the absorption coefficient is seen in **Figure 84** near the band edge in the MIR region. This is intuitive as low bandgap ϵ -Ge epi-layers are expected to have a higher absorption coefficient.

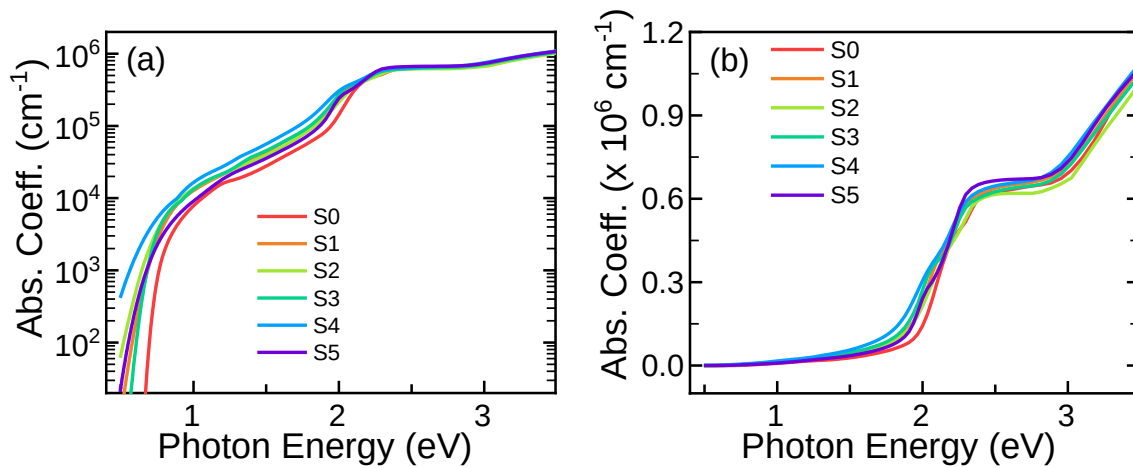


Figure 84. The absorption coefficient determined for the samples S0-S5 indicating a shift in the absorption spectra due to the tensile strain, (a) log scale and (b) linear scale.

Using Tauc's method, the absorption coefficient can be analyzed to determine the direct and indirect band edges in Ge and ϵ -Ge. This can be done by fitting the linear plot of the absorption coefficient *versus* the photon energy [39, 40]. However, this method comes with a degree of approximations and fitting-induced uncertainty [41]. We proceed to utilize this method to extract the band edge as the primary goal of this study is to highlight the change in the band structure and not to determine the exact values of the physical constants. The fitting is done while maximizing the R^2 fitting values for all samples and following an identical fitting process in the region where the absorption coefficient is 10^3 - 10^4 cm⁻¹ or higher [40]. **Figure 85** shows the raw fitting for the indirect band edge as well as the direct band edge extraction for visualizing Tauc's method for ϵ -Ge samples. It is evident from **Figure 85 (a)** that the indirect band edge lies in the vicinity of ~ 0.66 eV as expected at room temperature and moves to lower energies as tensile strain is applied.

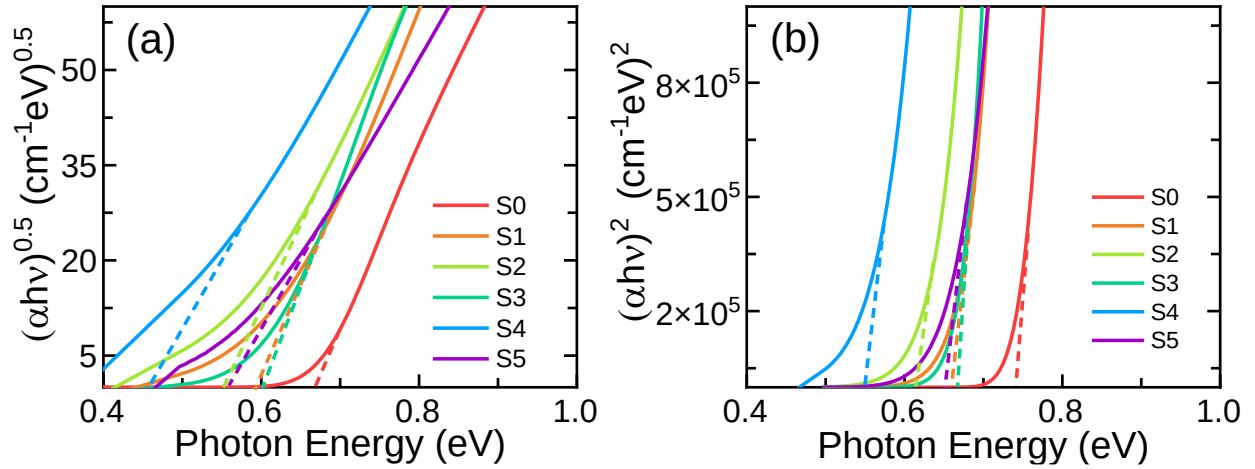


Figure 85. Using the Tauc's method to extract the approximate (a) indirect and (b) direct band edges for the samples as a function of tensile strain. The fitting while ensuring $R^2 \sim 0.99$ for all samples is overlaid on the curves. Due to the highly linear nature and R^2 often approaching 0.999, the error in the energy intercept is $< 1\text{meV}$.

Similarly, the direct band edge in **Figure 85 (b)** lies in the vicinity of $\sim 0.78\text{ eV}$ and moves to lower energies as tensile strain causes deformation of the bands.

Interestingly, it is possible to note a few consequential observations from comparing these band edges with the band movement known through theoretical $30 \times 30\text{ k.p}$ calculations for $\epsilon\text{-Ge}$ [1]. **Figure 86** highlights the various direct and indirect band edges as a function of tensile strain as well as the possible transitions in the band structure that could potentially cause them. Due to the broken degeneracy between the LH and HH bands, transitions are possible from both. Compared with k.p calculated band edge movement (see **Figure 86b**), it appears that indirect transitions prefer the L-LH transition over the L-HH as the latter one has an increasing transition energy. One possible explanation for this observed behavior could be the relative impact of JDOS and the transition energy (E_{tr}). Both these transitions have a large JDOS due to the large DOS of the L valley, so the differentiating factor becomes the transition energy E_{tr} . The transition rate depends linearly on the JDOS, but the dependence on the E_{tr} is exponential. Thus, although the L-HH transition will have a larger JDOS compared to L-LH, the difference is not sufficient to compensate for the exponential dependence on E_{tr} .

For the direct transitions associated with the Γ -valley and the LH or HH bands (see **Figure 86c**), the E_{tr} and the JDOS will impact the relative strength of each transition. It is clear from **Figure 86(d)** that the transitions take place from both potential paths, Γ -LH and Γ -HH as the solid

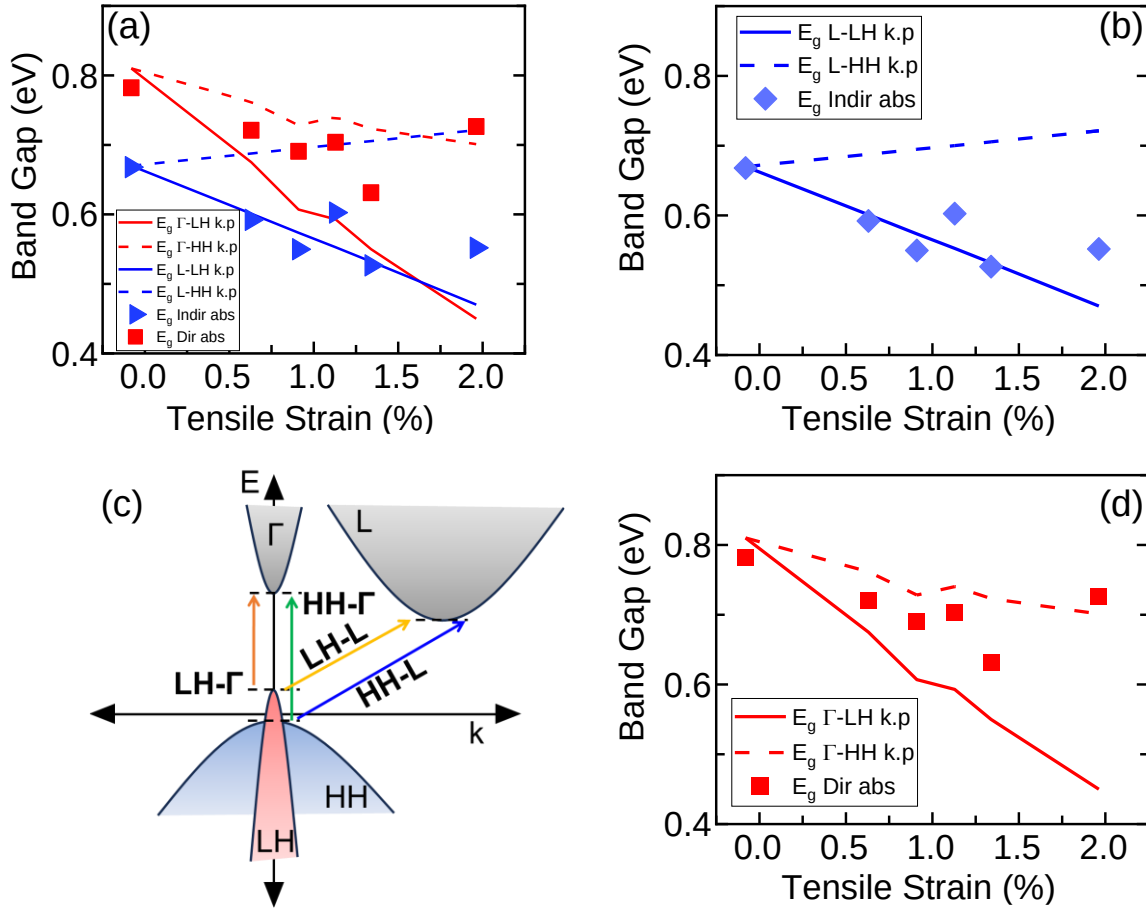


Figure 86. (a) The approximate direct and indirect bandgaps for the 6 samples S0-S5 as a function of tensile strain compared with the relative band edge shifts calculated to 30×30 k.p. (b) The indirect bandgap for the 6 samples indicating that the L-LH valley transition is dominant over the L-HH. (c) The 4 dominant transitions in this energy range are highlighted using a schematic. (d) the direct bandgaps measured for the 6 samples indicating a contribution from both Γ -HH and Γ -LH transitions with a mid-way trend. Here the solid data points are from VASE measurements.

data points (measured using VASE with Tauc's method) lie between the two predicted band edges for these transitions. Transitions from the LH band are initially insignificant as the JDOS is very low and the E_{tr} is the same as the HH transition. For the unstrained Ge, it is not possible to determine the origin of transitions (LH or HH) as the bands are degenerate. However, the transition rate for the Γ -HH transitions will have a much larger JDOS, hence it can be expected that the transitions are primarily originating from the Γ -HH coupling. As tensile strain is applied, the degeneracy is broken, and the LH transitions become exponentially more probable than HH

transitions. Thus, the observed direct band edges lie somewhere in between the two possible transitions as seen in *Figure 86(d)*.

6.7 Van-Hove singularities in Ge as a function of tensile strain

The absorption of light can be described as a direct electronic transition between two energy levels in the band structure or a transition assisted by the excitation of a phonon. Transitions are more probable where the joint electronic density of states shows a CP associated with a delta function $\delta(h\nu - E_{cp})$ in the JDOS. These inter-band transitions can be characterized using the numerical second-order derivative (see **Figure 87**) of the complex dielectric function versus the photon energy. The dielectric constant ($\epsilon_1 + i \epsilon_2$) as a function of the photon energy of Ge has a few specific inflection points in this energy range (0.5 eV to 4.1 eV) which can be enhanced using the second order derivative and linked to specific direct band transitions between various regions of the Brillouin zone. Such transitions have a fixed energy difference between the valence band (VB) and conduction band (CB), across many high-symmetry directions in the crystal structure of Ge and may not always relate to transitions between just a single pair of bands. This CP structure and the locations of various CPs in the band structure of Ge and ϵ -Ge are shown in **Figure 87** for 3 samples as an illustration of the ability of the 2nd order derivative of the dielectric functions to enhance the CPs. The numerical second-order derivative is calculated using the Stravitzky-Golay algorithm with a 5th-order polynomial interpolation between adjacent data points and a 10-point calculation window, stitched together to form the derivative spectra for the entire photon energy range.

Some general observations can be drawn from the trends seen in **Figure 87** : i) E_0 and $E_0 + \Delta_0$ CPs have a smaller transition amplitude compared to the others, ii) E_1 and $E_1 + \Delta_1$ CPs have the largest amplitude and the smallest broadening, iii) E_0' CP is the broadest with a large broadening factor, and iv) tensile strain moves all these CPs to lower energies. The CPs are extracted by fitting the derivative spectrum of the dielectric functions ϵ_1 and ϵ_2 simultaneously to the derivative of the complex Lorentzian [24, 25]. The fitting function has 4 parameters (E_{tr} , ϕ , Γ_B , and A) which are fit using a Levenberg–Marquardt algorithm for least square regression, ensuring an R^2 value tending to 1. The parameter E_{tr} is associated with the CP energy peak and is central to this study, ϕ , Γ_B and A are the phase, broadening factor, and amplitude of the CP, respectively. The complex Lorentzian function is fitted to the derivative of the dielectric function near the E_0 and $E_0 + \Delta_0$ CP such that [25],

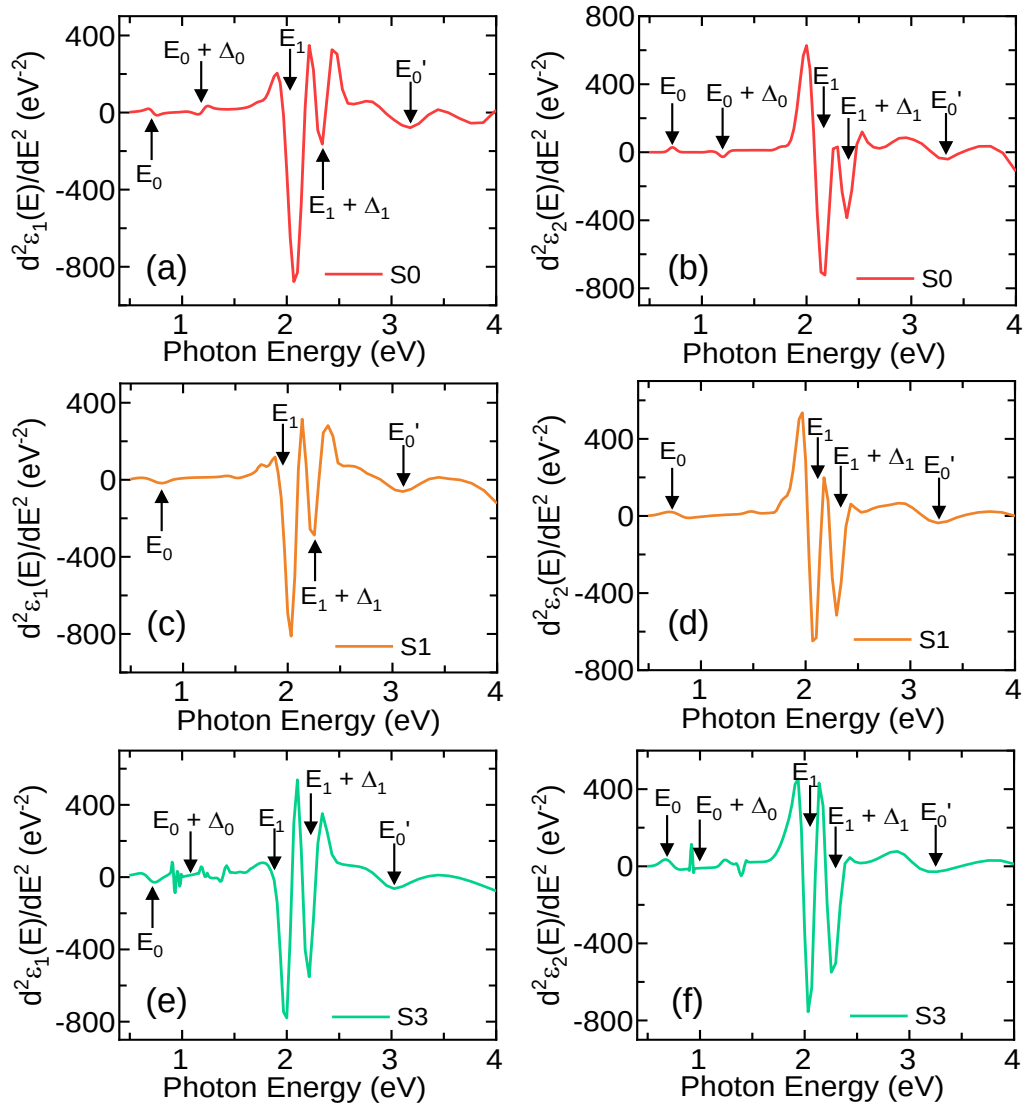


Figure 87. Van Hove singularities: the critical points have been shown for unstrained, moderately strained and highly strained samples using the second derivative of the dielectric functions. The extracted CP energies are shown for the 5 CPs visible in this range of the spectrum.

$$\frac{d^2 \varepsilon}{dE^2} = \frac{A_{E_0} e^{i\varphi}}{(E - E_0 + i\Gamma_{E_0})^{3/2}} . \quad (6.7.1)$$

Here, $\varepsilon = \varepsilon_1 + i \varepsilon_2$ is the complex dielectric constant. Similarly, the E_1 and $E_1 + \Delta_1$ CPs are fit simultaneously with the same expression for the two transitions. An additional fitting parameter Δ_1 (not to be confused with the Δ used to represent the measured ellipsometric angle in the earlier

section) is introduced in the fitting process to represent the spin-orbit coupling energy in the Λ direction. The E_1 and $E_1 + \Delta_1$ CP transitions are modeled using [25],

$$\frac{d^2\varepsilon}{dE^2} = \frac{A_{E_1} e^{i\varphi}}{(E - E_1 + i\Gamma_{E_1})^2}, \quad (6.7.2)$$

$$\frac{d^2\varepsilon}{dE^2} = \frac{A_{E_1 + \Delta} e^{i\varphi}}{(E - E_1 - \Delta + i\Gamma_{E_1 + \Delta})^2}. \quad (6.7.3)$$

The extracted CP energies as a function of tensile strain using the fitting process shown in Eqs. 6.7.1- 6.7.3 and second-order derivatives in **Figure 87** are summarized in **Figure 88 (a)-(d)** for the 5 CPs.

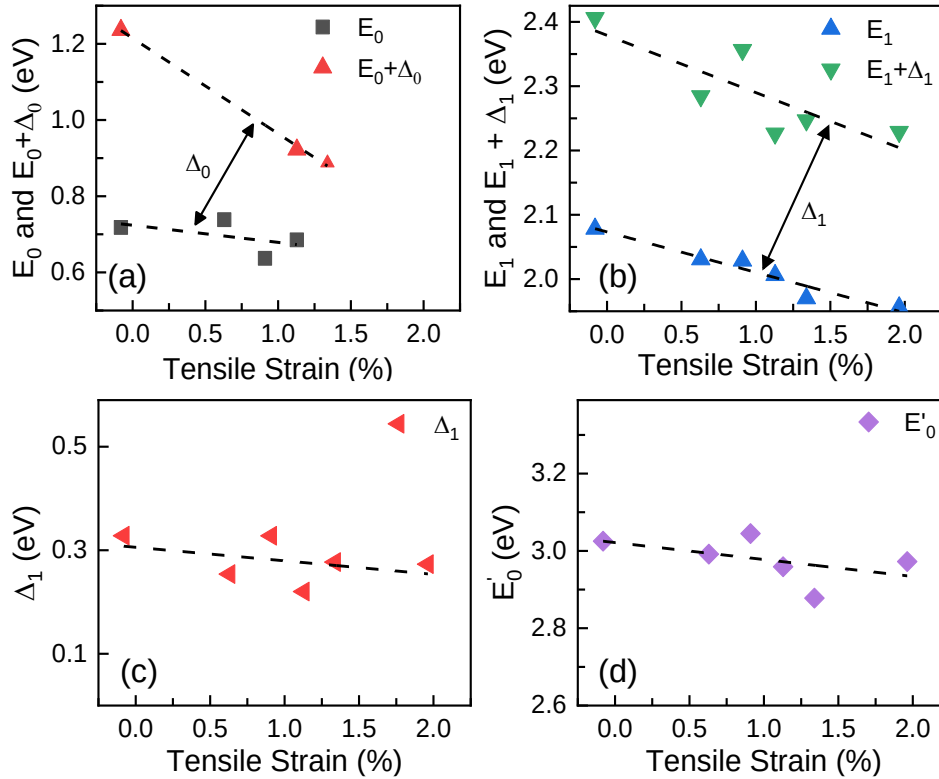


Figure 88. CP values as a function of strain in Ge layers. (a) The CP associated with the (a) fundamental band edge at E_0 and SO coupling $E_0 + \Delta_0$, (b) the E_1 and $E_1 + \Delta_1$ CP at the Λ -axis, (c) the SO energy Δ_1 obtained from the difference in the E_1 and $E_1 + \Delta_1$ CP, and (d) the E'_0 CP remaining nearly constant with applied tensile strain. The error in the CP energy peak after the fitting is of the order of ~ 2 meV for the E_0 peak, ~ 8 meV for the E_1 peak, and 25 meV for the E'_0 peak.

The CP associated with the direct gap E_0 is at the center of the Brillouin zone at the Γ -point, as a 3-dimensional minima M_0 . The CP near E_0 has the dielectric constant of the form $(E - E_0)^{0.5}$ in the absence of excitonic effects as is expected at room temperature. The E_0 transition is observed near the 0.5 eV - 0.8 eV spectral region and is directly linked to the fundamental band edge of Ge usually reported in the literature occurring between $\Gamma_{25'}$ - Γ_2' regions of the Brillouin zone. The CP E_0 determines most of the dielectric dispersion below the band edge since there are no other CPs below E_0 . The effect of epitaxial tensile strain can be understood as a perturbation resulting in a red shift of the E_0 CP, as seen in **Figure 88 (a)**. However, such a redshift into the MIR region moves closer to the end of the measurable range of the VASE equipment, and results in poor sensitivity for this transition for Ge samples with high tensile strain. Note that the E_0 and the band edge can be as low as ~ 0.45 eV for highly tensile strained samples used in this study, based on **k.p** estimates. The E_0 transition is thus detectable as a weak artifact only for the moderately strained samples and the unstrained Ge sample. Similarly, the $E_0 + \Delta_0$ CP associated with the SO coupling also follows a similar decreasing trend as seen in **Figure 88 (a)**. Although the number of extractable values of the $E_0 + \Delta_0$ and E_0 CP is not large as seen in **Figure 88 (a)**, due to the end of the measurable range in our current VASE setup, however, certain observations can be made. The SO energy Δ_0 , *i.e.*, the difference in the $E_0 + \Delta_0$ and E_0 CP energies, is seen to decrease with applied tensile strain in Ge, indicating that this apparent value of the SO coupling reduces

with tensile strain. Thus, it can be reasonable to expect that at a certain tensile strain value beyond $\sim 2.5\%$, the apparent SO coupling energy Δ_0 will tend to be zero or negative giving rise to interesting implications not yet known. Due to the broken degeneracy between the LH and HH bands by the strain, the E_0 CP should be seen as two distinct peaks, $E_0(1)$ and $E_0(2)$ associated with the transition to HH and LH, respectively. At room temperature, these CPs would be broadened and closely spaced resulting in the appearance of one single CP while being indistinguishable.

The behavior of the E_0 and $E_0 + \Delta_0$ CP with applied tensile strain can be visualized in **Figure 89(a)** which shows the split of the three transitions, indicated by arrows. By solving the

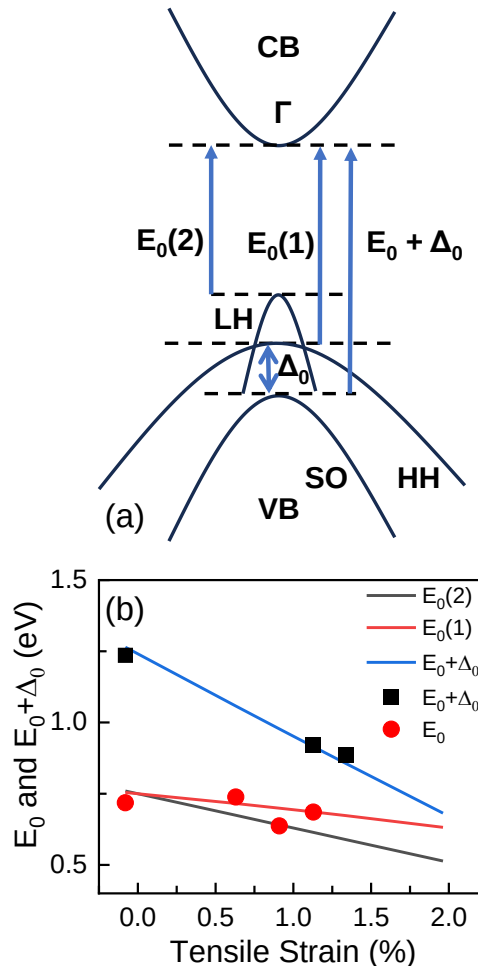


Figure 89. Understanding the E_0 CP behavior: (a) the three transitions possible after the broken degeneracy between the LH and HH bands due to the tensile strain, and (b) comparing the VASE extracted E_0 and $E_0 + \Delta_0$ CPs as a function of tensile strain, with theoretically predicted values using band theory calculations.

strain perturbed Hamiltonian including the hydrostatic and shear strain deformations of the CB, LH, HH, and SO bands, the changes in the three transitions can be computed up to the first-order approximation using [42],

$$\Delta(E_c - E_{LH}) = -\Delta E_H - \frac{1}{2}\Delta E_S \quad (6.7.4)$$

for the LH band $\left|\frac{3}{2}, \frac{3}{2}\right\rangle$ with ΔE_H representing the hydrostatic deformation of the band and ΔE_S representing the shear deformation. For the HH band $\left|\frac{3}{2}, \frac{1}{2}\right\rangle$, the impact of tensile strain can be expressed using,

$$\Delta(E_c - E_{HH}) = -\Delta E_H + \frac{1}{2}\Delta E_S - \frac{1}{2} \frac{(\Delta E_{S'})^2}{\Delta_0}. \quad (6.7.5)$$

Similarly, the SO band transition energy shift can be calculated using,

$$\Delta(E_c - E_{SO}) = \Delta_0 - \Delta E_{H'} + \frac{1}{2} \frac{(\Delta E_{S'})^2}{\Delta_0}. \quad (6.7.6)$$

The terms ΔE_H , ΔE_S , $\Delta E_{H'}$, and $\Delta E_{S'}$ are computed using the compliance constants and Ge 300 K material parameters from Ref. [43]. The deformation potential for the hydrostatic components $(C_1 + a)$ and $(C_1 + a')$ are assumed to be -10.9 eV and -11.2 eV, respectively. The shear deformation potentials b and b' are assumed to be -2.86 eV and -2.44 eV, respectively [42]. The tensile strain is assumed to be positive, and the expressions are modified accordingly as shown in Eq. 6.7.4 - 6.7.6.

The SO energy Δ_0 predicted in this measurement is slightly larger than reported in the literature [42]. The exact cause of this is unknown and could be a systemic shift in the measurement and fitting process, but the objective of this analysis is to highlight the impact of tensile strain on the relative CP energy trend between samples. The theoretical CP energies as a function of tensile strain are calculated using Eq. 6.7.4 - 6.7.6 (see **Figure 89(b)**) and are overlaid with the measured

CP energies for the E_0 and $E_0 + \Delta_0$ CP seen in this work. The unstrained SO energy Δ_0 is set at the same as the value measured for the unstrained sample S0, i.e., 0.45 eV. Although it is difficult to distinguish if the E_0 CP originates from the $E_0(1)$ or $E_0(2)$ transitions, they have a general decreasing trend aligning with the theoretical predictions. Furthermore, the reducing nature of the apparent SO energy Δ_0 is clear both in the measurements and the theoretical computations. We refrain from predicting the exact values of the SO energy Δ_0 as a function of tensile strain due to the sparse nature of the extractable CP energies in our study.

The artifacts associated with the E_1 and $E_1 + \Delta_1$ CPs are due to transitions between the top two VBs and the lowest CB along $\langle 111 \rangle$ direction in the Brillouin zone (Λ -axis). The E_1 CP is associated with the transitions between Λ_1 CB and the $\Lambda_{4,5}$ VB, whereas the $E_1 + \Delta_1$ CP is associated with the transition between the Λ_1 CB and the Λ_6 VB. Along this direction, the VB and CB are nearly parallel, represented by 2-dimensional minima in the band structure. The location and the dependence of the E_1 and $E_1 + \Delta_1$ CP energy on the tensile strain in Ge are shown in **Figure 88(b)**. The peak energy associated with this CP decreases with increasing tensile strain in Ge. The difference in the two trends is the SO energy Δ_1 , and a nearly fixed $\Delta_1 \sim 0.25$ eV can be observed even with increasing tensile strain in Ge. The value of the SO energy Δ_1 (see **Figure 88c**) is slightly larger than values usually reported in the literature of ~ 0.2 eV for Ge. This shift in the apparent value of the SO energy could be due to a strain-independent factor introducing a constant energy shift. The exact cause of this deviation is unknown at the time of writing this manuscript.

Further analysis of the E_1 and $E_1 + \Delta_1$ peak is possible based on the red shifting trend seen in **Figure 88(b)** to reveal some interesting mechanisms as the measured data is compared with the theoretical predictions. The impact of the SO coupling and the applied tensile strain is shown for the E_1 and $E_1 + \Delta_1$ peak in **Figure 90**. The shear and hydrostatic components of the strain have been separated, ΔE_s and ΔE_H , respectively. The hydrostatic deformation ΔE_H is calculated using [43],

$$\Delta E_H = \frac{2 D_1^1}{\sqrt{3}} \left(1 - \frac{c_{12}}{c_{11}} \right) \varepsilon_{out-of-plane}, \quad (6.7.7)$$

where c_{12} and c_{11} are the elastic constants, ε is the strain applied to the lattice and D_1^1 is the hydrostatic deformation potential for the CB at E_1 . The typical values of c_{11} and c_{12} 128.5 GPa and 48.3 GPa, respectively, are used in this analysis [43]. The strain is a fractional number of the order

of 0.01 and the hydrostatic deformation potential D_1^1 is -8.7 eV. The shear deformation of the VB can be calculated using [43],

$$\Delta E_s = -\sqrt{\frac{2}{3}} D_3^3 \left(1 + \frac{2c_{12}}{c_{11}}\right) \varepsilon_{out-of-plane}, \quad (6.7.8)$$

where the shear deformation potential for the E_1 VB is denoted by D_3^3 having a value of -5.6 eV. The out-of-plane strain $\varepsilon_{out-of-plane}$ can be computed by knowing the biaxial relaxation constant R_B where $\varepsilon_{out-of-plane} = -R_B \varepsilon_{in-plane}$. The applied tensile strain red-shifts the E_1 peaks as seen in **Figure 88 (b)**. The shifts in E_1 and $E_1 + \Delta_1$ peak can be theoretically computed using the following relation obtained by solving for the eigen energies of the strain Hamiltonian considering the SO coupling,

$$\partial(E_1)_t = \frac{\Delta_1}{2} - \Delta E_H - \frac{1}{2} \sqrt{\Delta_1^2 + 4(\Delta E_s)^2}, \quad (6.7.9)$$

$$\partial(E_1 + \Delta_1)_t = -\frac{\Delta_1}{2} - \Delta E_H + \frac{1}{2} \sqrt{\Delta_1^2 + 4(\Delta E_s)^2}. \quad (6.7.10)$$

Here, $\partial(E_1)_t$ and $\partial(E_1 + \Delta_1)_t$ indicate the difference of CP energy between the unstrained Ge and ε -Ge. The difference in the two peak energies associated with the “apparent” SO energy $(\Delta_1)_t$ can be obtained as,

$$\Delta_{1,t} = (E_1 + \Delta_1)_t - (E_1)_t = \frac{1}{2} \sqrt{\Delta_1^2 + 4(\Delta E_s)^2}. \quad (6.7.11)$$

It is evident that the apparent SO energy $\Delta_{1,t}$ will be amplified regardless of the type of strain applied, tensile or compressive, due to the squared dependence of the shear-induced energy shift. A simplification can be made by assuming that the shear-induced energy shift is much smaller than the SO energy Δ_1 , the expressions can be simplified by expanding the series to obtain,

$$\partial(E_1)_t = -\Delta E_H - \frac{(\Delta E_s)^2}{\Delta_1}, \quad (6.7.12)$$

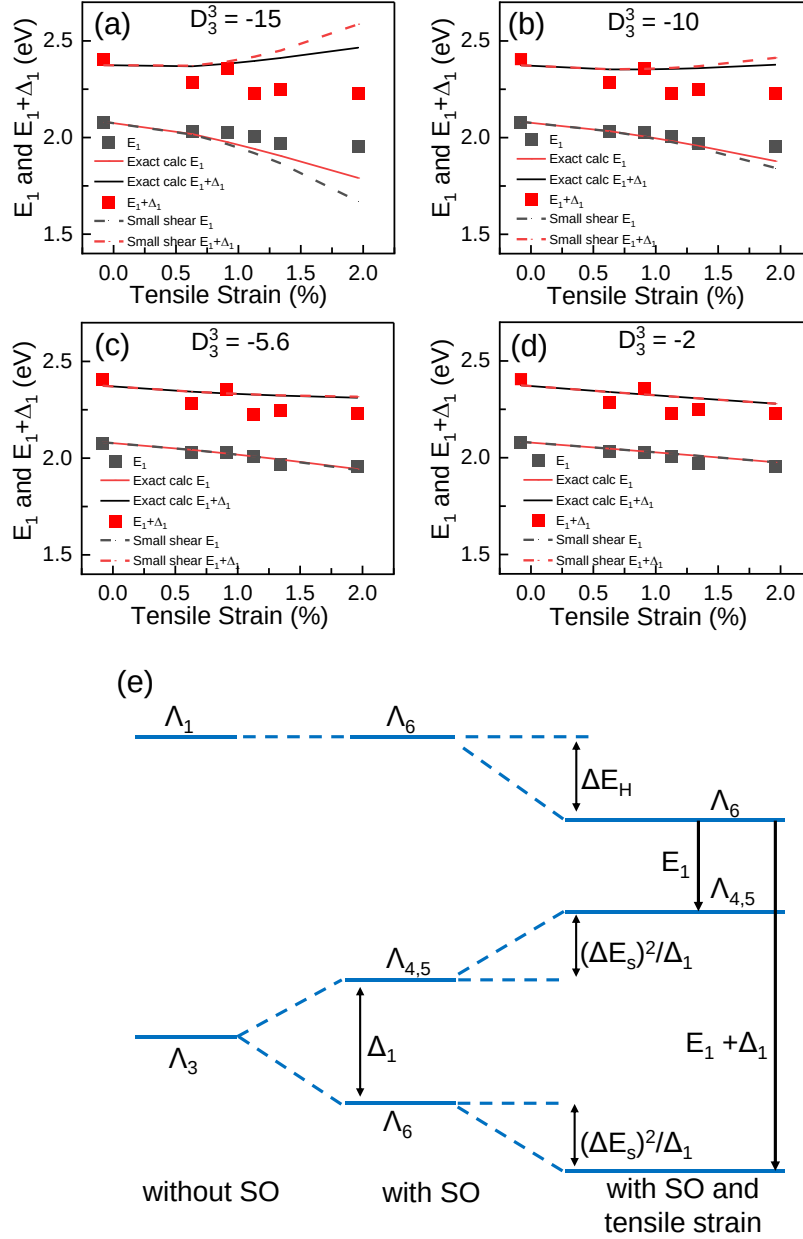


Figure 90. Understanding the E_1 CP behavior: Impact of the choice of shear deformation potential, (a) -15, (b) -10, (c) -5.6 and (d) -2 on the theoretically predicted value compared with the extracted VASE CP values. (e) Bands and corresponding transitions in the low shear approximation at the Λ axis for the E_1 CP.

$$\partial(E_1 + \Delta_1)_t = -\Delta E_H + \frac{(\Delta E_s)^2}{\Delta_1}. \quad (6.7.13)$$

This can further be used to obtain the simplified apparent SO energy $\Delta_{1,t}$ for tensile strained Ge,

$$\Delta_{1,t} = (E_1 + \Delta_1)_t - (E_1)_t = \Delta_1 + 2 \frac{(\Delta E_s)^2}{\Delta_1}. \quad (6.7.14)$$

The quadratic dependence of ΔE_s on the sign of the strain value, creates a shift that is again independent of the type of strain, i.e., tensile or compressive. This transition line-up discussed in Eq. 6.7.9 – 6.7.11 is schematically illustrated in **Figure 90** to show the E_1 and $E_1 + \Delta_1$ transition in the presence of SO coupling, tensile strain, and a small shear approximation.

To evaluate the validity of the exact equation described in Eq. 6.7.9 – 6.7.11 and the small shear expressions in Eq. 6.7.12 – 6.7.14, the predicted E_1 and $E_1 + \Delta_1$ transition are overlaid with these models. **Figure 90** shows the impact of low and high shear deformation potentials (-15 to -2) on the band edge movement compared to the VASE-extracted CP energies. While keeping the hydrostatic deformation potential D_1^1 fixed at -8.7 eV, **Figure 90(a), (b), (c), and (d)** vary the shear deformation potential D_3^3 to -15, -10, -5.6 and -2 respectively. The typically reported value of D_3^3 is -5.6 eV [43] and hence, **Figure 90(c)** has a better match between the predicted model values and the measured E_1 CP movement, compared to **Figure 90(a) and (b)**. A lower value of D_3^3 in **Figure 90(d)** agrees better than -5.6 eV with the E_1 CP data. A low shear deformation potential indicates a smaller shear component to the band movement, and a close agreement can be seen between the exact equation and the small shear approximation (*see Figure 90c and d*). It is evident that the low-shear approximation works best for the measured ε -Ge samples are presented in this work. This seems reasonable as the epitaxial strain amounts are below 2 % in this study. One can also notice that a threshold can be identified at ~ 1 % tensile strain where the shear approximation does not fit well with the data points for a large shear deformation potential D_3^3 of -10 eV or -15 eV (*see Figure 90a and b*). In the presence of a small shear deformation, looking at Eq. 6.7.14 the apparent value of the SO splitting $\Delta_{1,t}$ will have a negligible dependence on the value of ΔE_s and in extension, on the tensile strain ε . This explains the trend seen in **Figure 88(c)** which shows a nearly constant SO energy Δ_1 for increasing tensile strain as well as a parallel decreasing trend for the E_1

and $E_1 + \Delta_1$ peak. The impact of the hydrostatic and shear deformation on the various bands in Ge at the E_1 CP (Λ axis) in the presence of biaxial tensile strain is pictorially summarized in **Figure 90(e)** for the small shear approximation. In conclusion, we note that the epitaxial tensile strain applied to Ge thin films does not cause a large shear deformation of the VB at the E_1 CP (Λ axis), while maintaining a nearly fixed SO splitting energy Δ_1 with increasing tensile strain.

Lastly, the E_0' CP is seen as a broadened peak in **Figure 87** and a near-independence on the applied tensile strain is seen in **Figure 88(d)**. The broadened nature of the E_0' CP is due to many different regions contributing to these high energy transitions in the BZ and a mixing with the $E_0' + \Delta$ peak as well. Additionally, an analysis and interpretation for the broadening parameters as well as the Lorentzian amplitudes for all the CPs is possible similar to the CP energy trends shown in **Figure 87 and Figure 88**. But, this is further subject to additional fitting and measurement related deviations which can mask any real physical interpretation. Interestingly, the dielectric spectrum measured for some relaxed and bulk samples have been reported to have subtle differences in their respective spectrum. The presence of defects and dislocations is seen to be the cause, indicating that to a certain degree the CP structure can be used to gauge the material quality of the crystalline samples [43]. One potential indicator of relaxed/defective epi layer is the broadening of the E_1 CP [43]. The relatively un-broadened E_1 CP in this work can be a potential indicator of un-relaxed and non-defective Ge epi-layers.

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Chapter 7 – Lattice matched GeSn-InGaAs-InAlAs QW laser

7.1 Motivation and Scope: Lattice matched GeSn QW laser

Chapter 5 introduced a new type of Ge-based QW laser which utilized an InGaAs epitaxial layer as the waveguide as well as the strain template. The tensile strain imparted by this InGaAs layer on the Ge layer proved to be instrumental in producing optical transitions and gain. Further, it utilized quaternary layers on each side to provide confinement to the optical field forming the SCH structure. The controlled amount of tensile strain provided by the InGaAs layer onto the Ge QW proved to be beneficial in bringing down the threshold current from virtually impossible values to the $\sim 5 \text{ kA/cm}^2$ range. The adaptive waveguide design was seen to be crucial for waveguide design in this tunable laser stack for identifying the optimized operating wavelength where the net gain and threshold current density are good. However, a few places for improvement can be noticed:

- (i) Most III-V commercial lasers operate at much lower threshold currents $\sim 100 \text{ A/cm}^2$, can the Ge laser approach this value?
- (ii) Growth and processing of quaternary layers is cumbersome and prone to issues, a solution that by-passes this by using only ternary compounds will have value.
- (iii) Tensile strain improves the IQE, is better possible?
- (iv) Tensile strain may pose reliability challenges, can that be avoided?
- (v) IQE was also reduced due to Auger recombination, can that be bypassed?

This section explores, explains, and presents results for a GeSn-based QW laser that can achieve all improvements listed above (except (v)). These explorations are warranted considering the growing interest in germanium (Ge) and GeSn-based optoelectronic devices for applications beyond silicon (Si) transistors [1-3], optical components, detectors, and light sources [4-7] make a Ge-based monolithic photonic platform an interesting exploration. The recent rise in integrated quantum technologies can be accelerated if the diverse quantum components utilizing potentially

incompatible materials systems can be co-integrated heterogeneously using a chiplet-based approach [8]. This heterogeneous integration can be potentially simplified if the materials are Si-compatible or directly integrable on Si. Consequently, many reports over the last two decades have made tremendous progress in integrating Ge [9, 10], GeSn, and SiGeSn [11, 12] materials on Si to form optoelectronic devices.

The growth of GeSn directly on Si suffers from a large lattice mismatch, which causes defects and dislocations in the GeSn active layer [10], which can be inferred through the minority carrier lifetime [13]. Achieving a high carrier lifetime in the GeSn (or Ge) epitaxial layer is a key challenge in realizing efficient light sources [14] since defects become sites of non-radiative recombination. Interestingly, the GaAs material system ($\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$) due to its lattice proximity to $\text{Ge}_{1-y}\text{Sn}_y$ can provide lattice-matched or low-strain quantum well (QW) barriers and waveguide layers for a GeSn laser structure. Furthermore, the InAlAs/InGaAs/GeSn/InGaAs/InAlAs separate confinement heterostructure (SCH) QW structure is transferrable to a Si substrate *via* a graded buffer formed either with $\text{In}_x\text{Ga}_{1-x}\text{As}$ or $\text{In}_x\text{Al}_{1-x}\text{As}$ [4,13].

Implementing Ge-based light sources on Si is expected to be more challenging than conventional commercial III-V lasers, due to several key challenges:

- (i) Growth of device quality defect-free Ge or GeSn. Defects become centers of non-radiative recombination severely destroying IQE,
- (ii) sufficient band offsets to form type I carrier confinement.
- (iii) Refractive index step or gradient for optical confinement (SCH structure)
- (iv) In-direct bandgap nature of Ge or GeSn or SiGeSn and large density of states (DOS) in the L-valley resulting in lost carriers for radiative recombination.

Although integrating GeSn on Si directly using SiGeSn/GeSn heterostructure may provide extensive advantages such as:

- (i) manufacturability ease due to Si compatibility and Si know-how,
- (ii) use of simple Si-based binary and/or ternary alloys, and
- (iii) cost-benefit,

it is challenging to provide the key attributes required for efficient room temperature lasing listed above. Furthermore, the growth of GeSn on Si poses certain hurdles due to (i) increased lattice mismatch, (ii) low minority carrier lifetime due to lattice relaxation-induced defects, and (iii) low band offsets between the active and barrier layers leading to leakage of photons and electrons.

Historically, to achieve all the key attributes required for efficient room temperature lasing, the immensely successful commercial direct-gap III-V compound semiconductor-based lasers have employed complex layer stacks involving different compositions of ternary, quaternary, and penta-atomic layers [15-17]. Realizing GeSn light sources that perform efficiently comparable to direct gap light sources simply by utilizing the SiGeSn system might be “too good to be true”. We expect that similarly designed III-V layer stacks serving the purpose of lattice matching, lattice grading, lattice straining, refractive index grading, carrier confinement, and waveguiding will be required for achieving efficient lasing from the GeSn active layer. Direct-gap III-V materials can also be used in double heterostructure (DH) for light-emitting devices with realistic threshold current densities (J_{TH}), and QW structures can be formed to reduce the J_{TH} further [14,15] while improving tunability. But, for GeSn-based light sources, the indirect bandgap nature of GeSn at lower Sn alloy composition and high DOS of the L-valley mandate the use of QW structure to reduce the threshold current density to a realizable limit.

Through this section, we propose and analyze the use of $In_xGa_{1-x}As$ and $In_xAl_{1-x}As$ compositionally controlled epitaxial layers to form a separate confinement heterostructure (SCH) QW structure for the GeSn active layer. The key merit of this design is that the complete QW laser stack (GeSn QW, InGaAs waveguide, and barrier, InAlAs SCH layer, and contact layers) can be lattice-matched, resulting in no lattice-mismatched induced defects and potentially superior as well as reliable lasing performance. Additionally, the $In_xGa_{1-x}As$ and $In_xAl_{1-x}As$ layers can provide large band offsets with the GeSn layer to form a type I system with operability at room temperature. Furthermore, the lack of defects at the interfaces can mitigate any defect-induced band alignment changes [18] away from type I. The impact of Sn composition and the GeSn QW thickness on the key laser metrics such as bandgap energies, offsets, wavelength of emission, optical confinement factor, and waveguide design, are evaluated. The methodology of lattice matching $In_xGa_{1-x}As$ and $In_xAl_{1-x}As$ layers to compositionally controlled GeSn is examined to highlight the importance of tunability and design ease. Using TCAD solvers with material properties calibrated to Ge and

InGaAs [2,6], the 3D laser stack is evaluated using self-consistent numerical solvers to determine the potentials, currents, charge densities, fermi-levels, *etc* [6]. A custom gain solver is used to compute the QW laser performance metrics such as gain and J_{TH} [6], the details of which are discussed in Chapter 5. The proposed InAlAs/InGaAs/GeSn/InGaAs/InAlAs SCH laser structure can achieve an excellent J_{TH} approaching $\sim 10 \text{ A/cm}^2$ at an emission wavelength of $\sim 2.6 \mu\text{m}$ while providing good net modal gain for a single QW configuration of $\sim 40 \text{ cm}^{-1}$. As a consequence of Sn composition-dependent lasing wavelength, effective mass, bandgap, and conductivity of the stack, the proposed GeSn laser can perform optimally for Sn compositions between 8 - 18 %. Consequential implications of the GeSn/InGaAs QW system such as low joint-DOS, low effective mass, Γ - and L-valley energies and separation, quantum confinement, composition dependence, polarization dependence, and their impact on the lasing performance are discussed. Lastly, a lattice-mismatched modification to the GeSn/InGaAs QW laser structure is proposed that deviates marginally and controllably from the lattice-matched case. This controlled lattice mismatch can be engineered using the InAs composition in the waveguide. As the avenue of GeSn light sources evolves certain applications may demand a small degree of compressive or tensile strain in the GeSn active layer, similar to GeSn on SiGeSn system with added potential advantages. Furthermore, it may be challenging to obtain a perfect lattice-matched (or even a perfectly controlled strain) system in the real world although linearly graded buffer (LGB) has been studied extensively over the years. Hence, the possibility of controlling the In composition in graded InGaAs buffer can enable a “knob” to tune the lasing performance, offset the lattice mismatch or attain mismatch intentionally to enable appropriate lasing performance. This system has the potential to tune the optical and electrical characteristics while maintaining lattice matching in the entire laser stack, a desirable property that cannot be ignored.

7.2 Tunable application space for the GeSn Quantum well SCH system

This LM GeSn QW SCH laser has the potential to be an efficient, reliable, and tunable (1.2 μm to 6 μm wavelength) room-temperature light source, which can be monolithically integrated on a GaAs or Si substrate. The wide range of tunability of this GeSn QW laser as a function of Sn alloy composition and GeSn QW thickness is shown in **Figure 91**. Using the 30×30 **k.p** calculations for GeSn, the DOS effective mass and band energy trends are used in calculating the first few sub-band energies in the Γ -valley, LH-band, and HH-band. The InGaAs QW barrier height and thickness are determined through the adaptive waveguide design discussed below and in turn used to find the eigen energies in this finite QW system. Each transition according to Fermi's golden rule is evaluated, obtaining higher transition strength for the HH-band transitions owing to the larger DOS of the HH-band. The emission wavelength in **Figure 91** is the difference

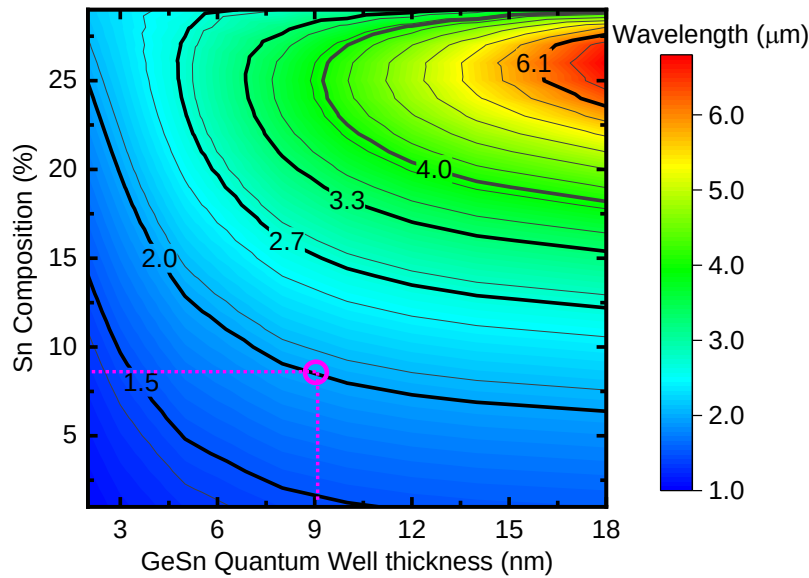


Figure 91. Large tunability (1.2 μm to 6 μm wavelength) of the proposed GeSn/InGaAs/InAlAs SCH QW laser structure as a function of the Sn composition in GeSn QW and the QW thickness. A sample design point is marked for lasing operation at a wavelength of 2 μm considering the HH-band to Γ -valley ground state sub-band transition.

in the sub-band energies for the HH-band to Γ -valley transition in the GeSn QW. Similar wavelength peaks (compared with **Figure 91**) have been observed in various studies over the years for GeSn, as part of theoretical and experimental studies: emission at ~ 2.2 μm for Sn 11 % [12], ~ 2.7 μm at Sn = 13 % [12] and ~ 2.8 μm at Sn = 16 % [19]. The other possible emission peaks

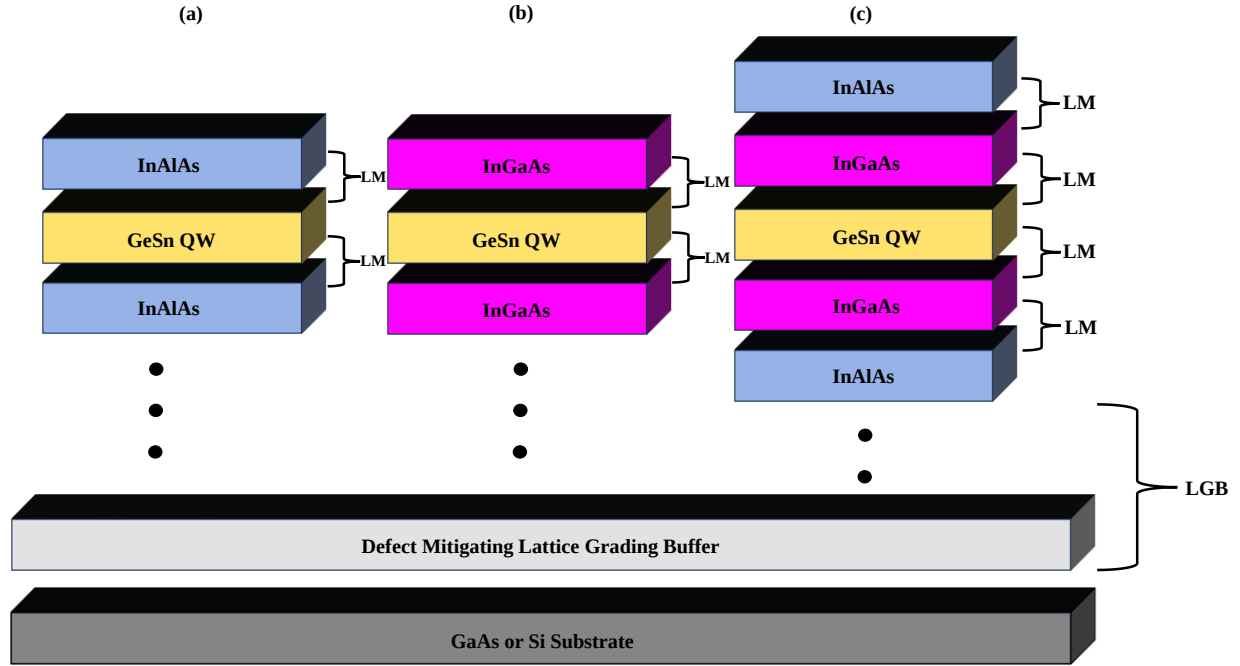


Figure 92. Three LED/Laser architectures possible using this material system leveraging the benefits of lattice matching.

are discussed in later sections. Particular wavelength contours for important applications are highlighted such as optical communication at $1.5 \mu\text{m}$ and extended-spectrum for fiber communication at $2 \mu\text{m}$ [20], gas sensing C-H stretch at $3.3 \mu\text{m}$ [21], and missile defense. The proposed system can have a wide range of applications such as daytime quantum key distribution (QKD) [22], integrated Si optics and quantum sensing [23, 24], and probing of gas molecules [25].

Schematic representations of the three proposed GeSn QW laser structures are shown in **Figure 92**, where only the substrate and the QW waveguide regions are represented. Each of the structures can be grown on a GaAs or Si substrate *via* a lattice grading $\text{In}_x\text{Ga}_{1-x}\text{As}$ or $\text{In}_x\text{Al}_{1-x}\text{As}$ buffer to translate the lattice constant to the desired Sn composition in GeSn QW while mitigating the defects and dislocations in the active layer. The structures will then involve p- and n-type doped regions, which provide the carriers for injection into the GeSn QW. This growth of GeSn QW structures is realized through vacuum interconnected dual chamber solid source molecular beam epitaxy. The proposed design shown in **Figure 92(a)** involves GeSn sandwiched between two LM $\text{In}_x\text{Al}_{1-x}\text{As}$ layers to form the GeSn QW. Such a structure is expected to provide very high band offsets and is thus suitable for high-temperature operation. Similar GeSn/ $\text{In}_x\text{Al}_{1-x}\text{As}$ structures

have previously been grown, characterized, and reported in Ref. 26. This structure can be further enhanced (better optical confinement) to have a SCH structure for the $\text{Ge}_{1-y}\text{Sn}_y$ QW by utilizing AlGaInAs quaternary layers as cladding, similar to Ge SCH QW reported in Ref. 6. Furthermore, the direct molecular beam epitaxy (MBE) growth of Ge or GeSn on $\text{In}_x\text{Ga}_{1-x}\text{As}$ is preferred over $\text{In}_x\text{Al}_{1-x}\text{As}$ due to surface higher surface roughness of InAlAs than InGaAs where the ad-atom surface mobility of aluminum is lower than gallium. Consequently, the next proposed GeSn QW laser structure shown in **Figure 92(b)** utilizes a $\text{GeSn}/\text{In}_x\text{Ga}_{1-x}\text{As}$ heterostructure. This structure provides good band offsets, sufficient for room temperature operation with a relative growth advantage of lattice-matched $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layer. Finally, for enhanced optical confinement the structure can be modified as shown in **Figure 92(c)** to include an $\text{In}_x\text{Al}_{1-x}\text{As}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GeSn}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_x\text{Al}_{1-x}\text{As}$ SCH QW structure. The SCH for optical confinement is essential for lasing activity, hence **Figure 92(a)** and **Figure 92(b)** can be LED architectures. Since all 3

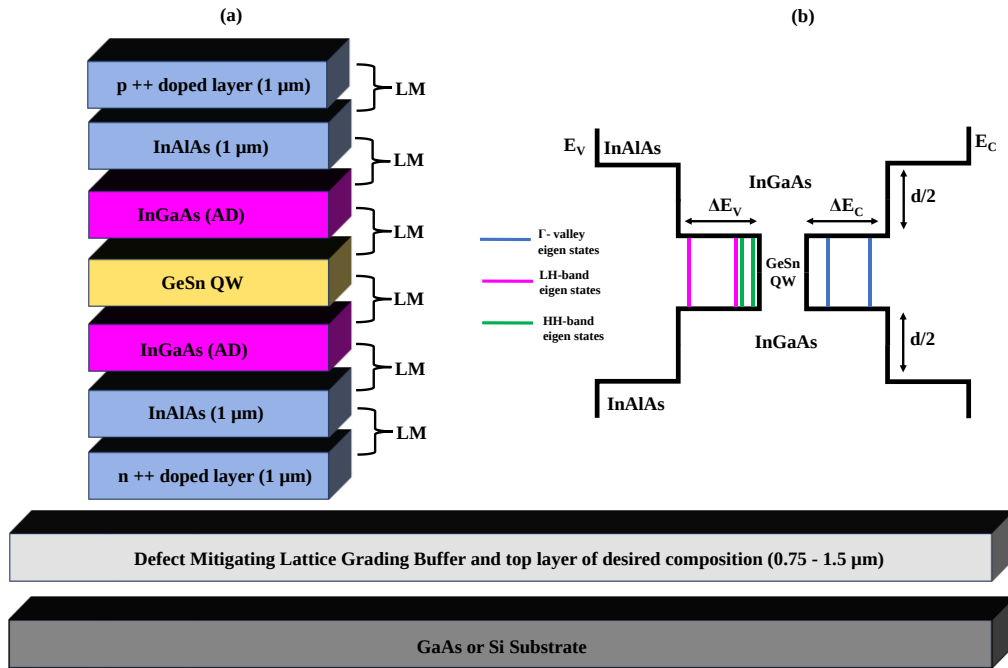


Figure 93. GeSn QW laser and SCH waveguide structure which utilizes a lattice matched stack (i.e., each of the heterointerfaces is LM) grown on a GaAs or Si substrate. The LM GeSn laser waveguide simulation structure (a) GeSn/ $\text{InGaAs}/\text{InAlAs}$ SCH QW grown on a GaAs substrate and transferrable to Si and (b) the corresponding schematic band structure associated with the SCH QW. The acronym AD is shown for the InGaAs waveguide layers to indicate that the thickness is chosen according to the adaptive design methodology to adapt and optimize the optical confinement factor to the changing emission characteristics.

structures were LM, the constraint of the critical layer thickness [18] is eliminated resulting in better design flexibility, reliability, fewer defects, and reduced free carrier absorption.

A schematic representation of the proposed GeSn QW SCH laser structure, the focus of this work, is shown in **Figure 93**, which also represents the sample structure used for simulations and predictions in this work. The LGB design and implementation are crucial for the proposed laser structure as the LGB is expected to contain a dense network of misfit defects while attaining the desired InAlAs or InGaAs composition from the GaAs substrate. Once the desired composition in the LGB is reached, the layer is topped off with a thick layer of the desired composition InGaAs or InAlAs to ensure that the lasing active region is further away from the LGB defects and is truly relaxed. For systems where the LGB did not relax completely resulting in small residual strains such as 0.1 %, the critical layer thicknesses are very large approaching the micrometer range, exponentially. In this case, the strain relaxation-induced defects are a very small concern. We have demonstrated such fully relaxed InGaAs/InAlAs LGB in the past for many compositions of InGaAs and InAlAs buffers [4, 10, 13, 26], the methodology to do so has been well studied over the years. The structure will then involve p - and n -type doped regions outside the SCH structure, which provide the carriers for injection into the GeSn QW. This growth of GeSn QW structures is realized through vacuum interconnected dual chamber solid source molecular beam epitaxy (MBE) [13, 26]. The proposed design shown in **Figure 93(a)** involves GeSn sandwiched between two LM $\text{In}_x\text{Ga}_{1-x}\text{As}$ layers to form the GeSn QW laser structure. The $\text{In}_x\text{Al}_{1-x}\text{As}$ layers form the SCH for confining the optical field thus enhancing the optical confinement factor through a large refractive index step. This structure utilizes a GeSn-on- $\text{In}_x\text{Ga}_{1-x}\text{As}$ heterointerface which is expected to provide good band offsets for carrier confinement. Since the $\text{In}_x\text{Al}_{1-x}\text{As}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GeSn}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_x\text{Al}_{1-x}\text{As}$ SCH QW structure is LM, the constraint of the critical layer thickness [18] is eliminated resulting in better design flexibility, reliability, fewer defects, higher carrier lifetime, and reduced free carrier absorption. Furthermore, limiting the relaxation-induced defects far away from the SCH lasing structure and within the LGB will benefit device performance regarding internal quantum efficiency (IQE) and band alignment [6, 14]. Eliminating the critical layer thickness limit for this laser stack also opens avenues for exploring multiple QW (MQW) structures based on GeSn. **Figure 93(b)** shows the schematic representation of the band structure of the $\text{In}_x\text{Al}_{1-x}\text{As}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{GeSn}/\text{In}_x\text{Ga}_{1-x}\text{As}/\text{In}_x\text{Al}_{1-x}\text{As}$ SCH QW structure. The various design metrics under consideration in this work are denoted in **Figure 93(b)** such as (i)

band offsets ΔE_C and ΔE_V , (ii) waveguide thickness $d/2$, and (iii) the electron and hole eigenstates in the CB and VB. The waveguide thickness $d/2$ is dependent on the Sn and In composition, corresponding refractive indices, and emission wavelength, and is chosen through an adaptive design methodology to optimize the optical confinement factor [6].

7.3 Lattice matching in the GeSn Quantum well SCH system

Sn alloying [11, 13, 26] and epitaxial tensile strain [4, 6, 9] are two techniques used to transition Ge to a direct bandgap material and make it an efficient light source. Both these techniques have certain challenges and drawbacks. For example, GeSn alloys pose processing/fabrication challenges as well as Sn clustering and segregation issues. Whereas the tensile Ge system has a certain critical layer thickness beyond which the strain field relaxes completely and creates defects and dislocations. In GeSn, the Sn alloying effect lowers the Γ -valley making GeSn a more direct bandgap active layer, but the presence of any compressive strain pushes the Γ -valley upwards resulting in a partial negation of the benefits of Sn alloying, *i.e.*, masking of the Sn-alloying beneficial effect. Interestingly, it is predicted that GeSn on Ge heteroepitaxial growths may never transition to a direct bandgap nature for any composition of Sn due to the compressive strain [28], and a similar trend can be expected for GeSn on GaAs or AlAs.

Lattice matching of the $\text{Ge}_{1-y}\text{Sn}_y$ QW with the SCH structure has certain benefits such as: (i) no critical layer thickness limit on GeSn layers creating ease for an arbitrary number of QWs, (ii) no strain field and strain relaxation induced defects, (iii) absence of compressive strain in GeSn avoids masking of Sn effect while preserving the energy separation between the Γ - and L-valley,

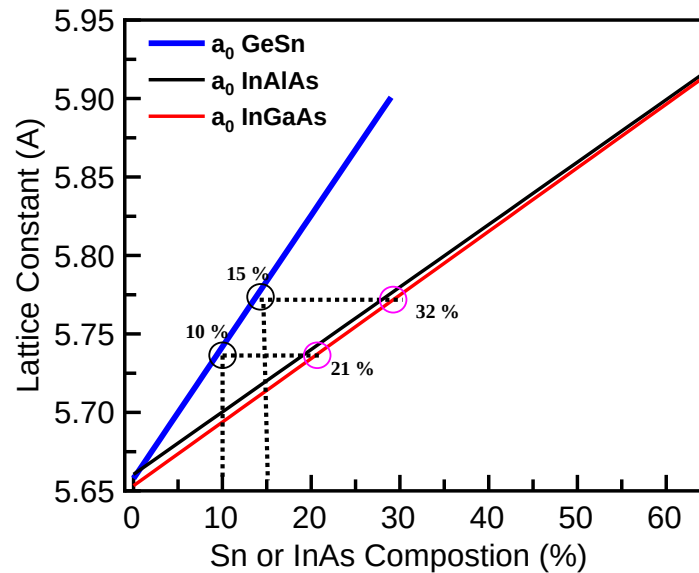


Figure 94. The lattice constants of the 3 materials, GeSn, InGaAs and InAlAs which form the proposed lattice matched GeSn QW SCH laser as a function of their alloy compositions. For a given Sn composition in GeSn, by approximately doubling the InAs composition in the InGaAs (or InAlAs) waveguide layer or barrier layer, one can achieve lattice matching.

(iv) better material quality and interfaces indicated through a high minority carrier lifetime, (v) higher band offsets and refractive index step, and (vi) improved IQE due to reduced non-radiative recombination. The radiative carrier recombination takes place in the GeSn active layer and the LGB defects are nearly 3 μm away from the GeSn layer, *see Figure 93*. Also, there is a large refractive index step between the InGaAs and the InAlAs SCH ($\Delta n \sim 0.3$), sufficient to confine a large fraction of the electric field within the waveguide, with a negligible amount reaching the LGB. The impact of the LGB defects on the optical field and emission is thus assumed to be ignorable in this simulation framework, due to the LGB growth relaxation know-how and distance from the active region. Recently, $\text{Ge}_{0.94}\text{Sn}_{0.06}$ samples were grown using the MBE system on a lattice-matched $\text{In}_{0.12}\text{Al}_{0.88}\text{As}$ underlayer [26]. Due to the lattice-matched interface, the minority carrier lifetime measured through the microwave photoconductive decay ($\mu\text{-PCD}$) technique was as high as 300 ns, indicating a good material quality and a drastically reduced Shockley–Read–Hall recombination, which would result in improved IQE [6, 14].

The adaptive methodology for lattice matching and composition choice of the waveguide and cladding layers formed by $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ is summarized in *Figure 94*. For example, choosing Sn composition of 10 % in $\text{Ge}_{1-y}\text{Sn}_y$, one must set the InAs mole-fraction in $\text{In}_x\text{Ga}_{1-x}\text{As}$ (the QW barrier and waveguide) and $\text{In}_x\text{Al}_{1-x}\text{As}$ (the SCH cladding) layers in the laser stack at nearly 21 %. Note that the composition is slightly different for $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ due to the small difference in lattice constants. In essence, the InAs composition in $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ must be about double that of the Sn composition in $\text{Ge}_{1-y}\text{Sn}_y$, ensuring lattice matching *i.e.*, equal lattice constants for the two materials,

$$\text{For LM : } a(\text{Ge}_{1-y}\text{Sn}_y) \approx a(\text{In}_{2y}\text{Ga}_{1-2y}\text{As}) \approx a(\text{In}_{2y}\text{Al}_{1-2y}\text{As}) \quad (7.3.1).$$

The choice of Sn composition will depend on many aspects such as the wavelength of emission, IQE, gain, J_{TH} , gain, application requirement, *etc.*, and the InAs composition will be set correspondingly based on the Sn composition, shown in *Figure 95(a)*. Once lattice matched to the choice of Sn composition in $\text{Ge}_{1-y}\text{Sn}_y$, the bandgaps of the 3 LM materials $\text{Ge}_{1-y}\text{Sn}_y$, $\text{In}_x\text{Ga}_{1-x}\text{As}$, and $\text{In}_x\text{Al}_{1-x}\text{As}$ are now dependent on the Sn composition as shown in *Figure 95(b)*. The transition point where $\text{Ge}_{1-y}\text{Sn}_y$ transitions to a direct bandgap material is visible as the intersection of the L- and Γ -valley energies at $\sim 8\%$ Sn. The SCH structure (see *Figure 93*) was chosen for the $\text{Ge}_{1-y}\text{Sn}_y$

QW as it provides good optical confinement through a refractive index step. It can be seen through **Figure 95(b)** that the bandgaps of $\text{Ge}_{1-y}\text{Sn}_y$, $\text{In}_x\text{Ga}_{1-x}\text{As}$, and $\text{In}_x\text{Al}_{1-x}\text{As}$ were in increasing order of energy when all three layers were lattice matched for all Sn compositions. This implies that the refractive index would be in the decreasing order thus creating the required SCH step profile for confining the optical field within the waveguide, with InAlAs having the lowest refractive index. Although the exact band alignment of the $\text{Ge}_{1-y}\text{Sn}_y/\text{In}_x\text{Ga}_{1-x}\text{As}$ interface as well as its composition dependence is not known, the total available band offset for this virtually defect-free interface can be estimated as shown in **Figure 95(c)**. The total band offset is the difference in the bandgaps of $\text{Ge}_{1-y}\text{Sn}_y$ and $\text{In}_x\text{Ga}_{1-x}\text{As}$ or $\text{In}_x\text{Al}_{1-x}\text{As}$ at the corresponding LM composition. It is evident that at all Sn compositions, the proposed $\text{Ge}_{1-y}\text{Sn}_y$ SCH QW laser structure can provide large band offsets and a step profile of bandgaps suitable for SCH.

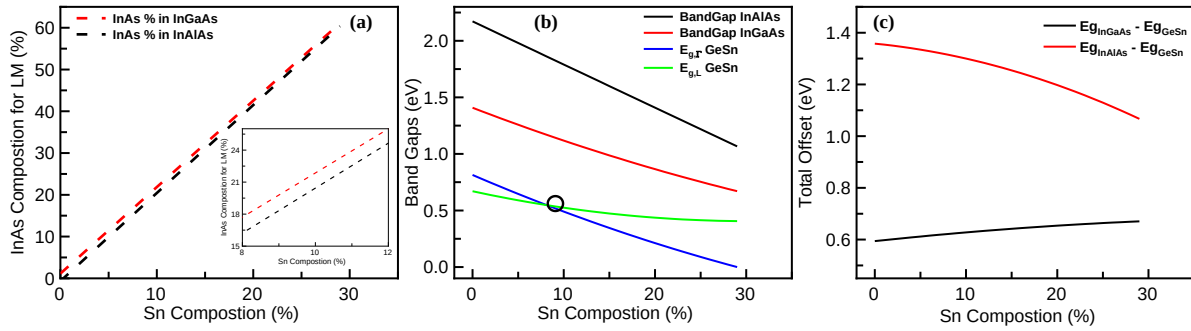


Figure 95. Lattice matching methodology in the GeSn QW laser stack as a function of Sn composition in GeSn QW: (a) The InAs composition required in the InAlAs barrier layer and InGaAs waveguide layer to achieve lattice matching, and (b) the corresponding bandgaps of the 3 materials in the lattice matched SCH QW stack. (c) the total available band offset for the $\text{Ge}_{1-y}\text{Sn}_y$ LM SCH QW laser stack.

7.4 GeSn SCH QW system: Adaptive Waveguide design

One critical problem in the design of this tunable wavelength GeSn laser is that the waveguide needs to adapt to the emission wavelength dynamically to optimize the optical confinement factor and reduce the material losses. More details about this methodology are discussed in Chapter 5 for the tensile Ge laser. The adaptive design methodology is used to arrive at the thickness and composition numbers for the structure shown in **Figure 93(a)**, to optimize the optical confinement ensuring a larger overlap of the QW with the E-field. For operation at $2.8\ \mu\text{m}$, the Sn composition must be $\sim 15\%$, consequently, the InGaAs (and InAlAs) composition to be $\sim 30\%$. Now that the compositions, bandgaps, and refractive indices of the waveguiding layers are known, the choice of InGaAs thickness is crucial and is discussed including the adaptive design in **Figure 96(a)**. For a choice of Sn $\sim 15\%$, the waveguide thickness of InGaAs on each side must be $\sim 350\text{nm}/2$ i.e., 175 nm . The optical confinement factor has an inflection point at this chosen

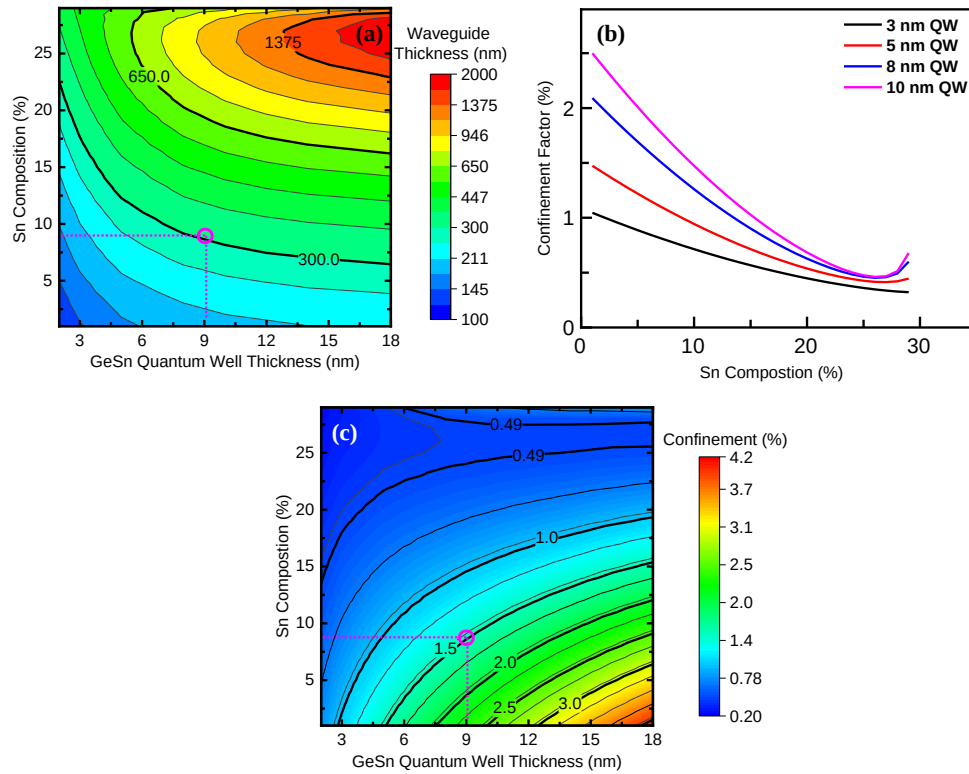


Figure 96. $\text{Ge}_{1-y}\text{Sn}_y/\text{In}_x\text{Ga}_{1-x}\text{As}$ LM SCH QW waveguide properties as a function of Sn composition: (a) optimum $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide thickness needed to achieve the optimum confinement factor when $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{Ge}_{1-y}\text{Sn}_y$ are LM. (b) and (c) optimum confinement factor of the GeSn QW as a function of Sn composition and GeSn QW thickness.

value and choosing a waveguide thickness above or below this would provide a drastically lower confinement factor [6]. Now if one chooses a Sn composition and chooses the right waveguide thickness based on the adaptive design, the best confinement factor can be obtained. This optimal confinement factor obtainable through adaptive design is shown in **Figure 96(b)**. Although the structure will house many optical modes for the E-field (TE as well as TM), this analysis only includes the fundamental TE and TM modes in the optical solver. The recombination from the HH band largely produces TE emissions, whereas the recombination from the LH band produces TM emissions, this is determined by the transition strengths in the GeSn QW [6, 28]. The actual mode propagation will be quasi-TE or quasi-TM with a mix of many modes.

The emitted optical field confined in the 3-slab waveguide, the Sn composition in the $\text{Ge}_{1-y}\text{Sn}_y$ QW as well as the QW thickness will affect the confinement factor [6]. As the Sn composition in the $\text{Ge}_{1-y}\text{Sn}_y$ QW is increased, the emission wavelength increases while also affecting the refractive indices of the layers in the SCH waveguide. At longer wavelengths, confining the optical field within the waveguide (*i.e.*, with a large optical confinement factor) becomes challenging. This is because, the refractive index of the InGaAs waveguiding layers confining the wave reduces, resulting in a smaller SCH refractive index step (Δn) between the waveguide and the SCH cladding, and consequently poorer optical confinement. A large refractive index step means better optical confinement. Using the adaptive design [6], the waveguide thickness (d , *see Figure 93*) is optimized in all scenarios to get the best possible confinement factor even with a reduced refractive index step, *see Figure 96*. Upon proper waveguide design [6], the maximum optical confinement factor attainable as a function of Sn composition is shown in **Figure 96(b)** for various QW thicknesses. For optimal waveguide design corresponding to the Sn composition, the $\text{In}_x\text{Ga}_{1-x}\text{As}$ composition must be LM to $\text{Ge}_{1-y}\text{Sn}_y$, as discussed in **Figure 95(a)** and the thickness of the waveguide shown in **Figure 96(a)** must be selected. The thickness d shown in **Figure 96(a)** is the total optimal thickness of the $\text{In}_x\text{Ga}_{1-x}\text{As}$ waveguide, *i.e.*, the $\text{Ge}_{1-y}\text{Sn}_y$ QW will be sandwiched between two $\text{In}_x\text{Ga}_{1-x}\text{As}$ layers of thickness $d/2$. The thicknesses $d/2$ of the InGaAs waveguide are denoted in **Figure 93(b)**. **Figure 96(b)** and **(c)** summarize the design space while highlighting the interdependent impact of the QW thickness and Sn composition on the $\text{Ge}_{1-y}\text{Sn}_y$ SCH QW laser structure. A sample design point with a Sn composition of $\sim 9\%$ and a QW thickness of 9 nm is marked in **Figure 96(a)** and **(c)** as well as in **Figure 91**. This $\text{Ge}_{1-y}\text{Sn}_y$ QW SCH structure will operate at $\sim 2\ \mu\text{m}$ wavelength and the cavity would have a confinement factor of 1.5 % provided

the waveguide is designed at the optical cavity thickness of $d = 300$ nm. At Sn compositions beyond 7-8 %, $\text{Ge}_{1-y}\text{Sn}_y$ transitions to a direct bandgap material and thus can provide relatively efficient lasing, making higher Sn compositions desirable. However, the Sn composition also affects the emission wavelength for the specific applications making the choice of Sn composition crucial.

7.5 Impact of Sn composition of k.p band structure and band alignment

As the $\text{Ge}_{1-y}\text{Sn}_y$ SCH QW is formed, the ground state eigen energies move to higher values, and the effective bandgap of the $\text{Ge}_{1-y}\text{Sn}_y$ QW is now larger than the bulk bandgap of $\text{Ge}_{1-y}\text{Sn}_y$. The impact of QW thickness on the quantization of energy levels and consequently the effective bandgap is shown in **Figure 97(a)** as a function of Sn composition in the $\text{Ge}_{1-y}\text{Sn}_y$ QW. The corresponding emission wavelength as a function of Sn composition in the $\text{Ge}_{1-y}\text{Sn}_y$ QW is shown in **Figure 97(b)**. Alloying with Sn produces a drastic reduction in the effective mass of the Γ -valley electrons in the CB as well as the LH-band which impacts the emission wavelength as seen in **Figure 97(b)**. The impact of $\text{Ge}_{1-y}\text{Sn}_y$ composition-dependent quantization can be understood through **Figure 97(c)**, which shows the impact on the effective bandgap beyond the bulk $\text{Ge}_{1-y}\text{Sn}_y$ bandgap. It is important to note that the emission from the $\text{Ge}_{1-y}\text{Sn}_y$ QW occurs largely from the Γ – HH transition resulting in transverse electric (TE) dominant emission [6, 28]. Emissions involving the LH-band, although nearly degenerate with the HH-band would have a smaller gain

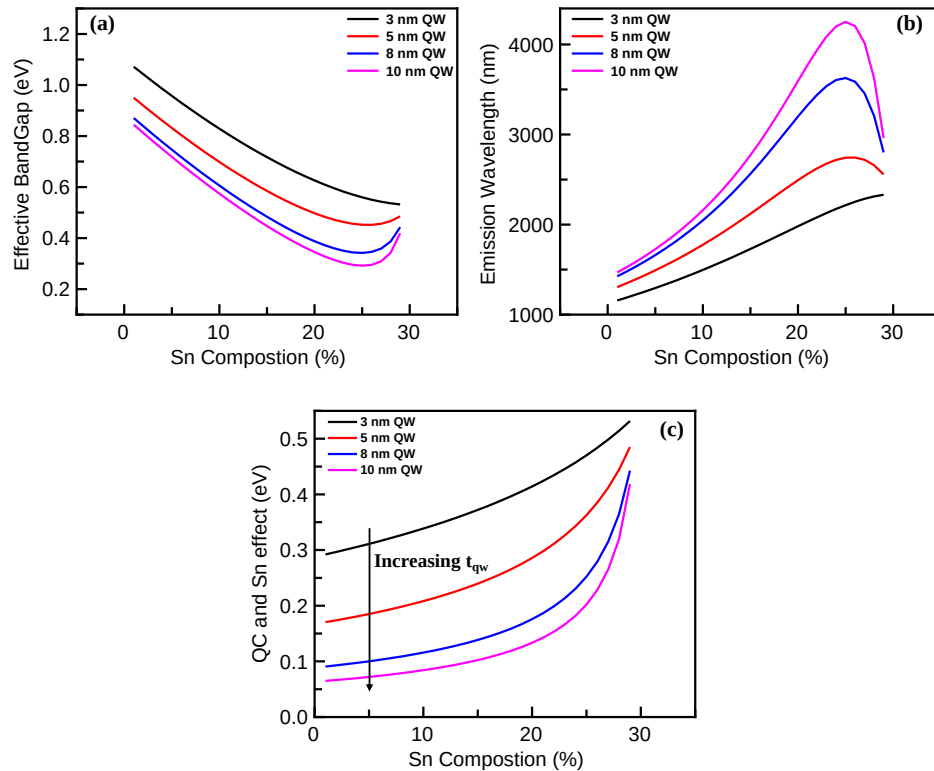


Figure 97.(a) Effective bandgap of $\text{Ge}_{1-y}\text{Sn}_y$ QW as a function of Sn composition, (b) corresponding transverse electric (TE) emission wavelength and (c) impact of Sn alloying and quantization on the effective band edge as a function of Sn composition.

as the DOS of the LH-band is low [6]. Radiative emissions from the L-valley are unlikely and negligible compared to the transitions from the Γ -valley, but the impact of the large L-valley DOS on the carrier densities is significant here while affecting the J_{TH} [6, 29].

To estimate the valence band offset (VBO) and conduction band offset (CBO), certain assumptions need to be made regarding the VBO since no experimental results for compositional dependence of the $\text{Ge}_{1-y}\text{Sn}_y/\text{In}_x\text{Ga}_{1-x}\text{As}$ band alignment are available. X-ray photoelectron spectroscopy measurement of Ge/GaAs structure was reported in Ref. 30 previously to determine

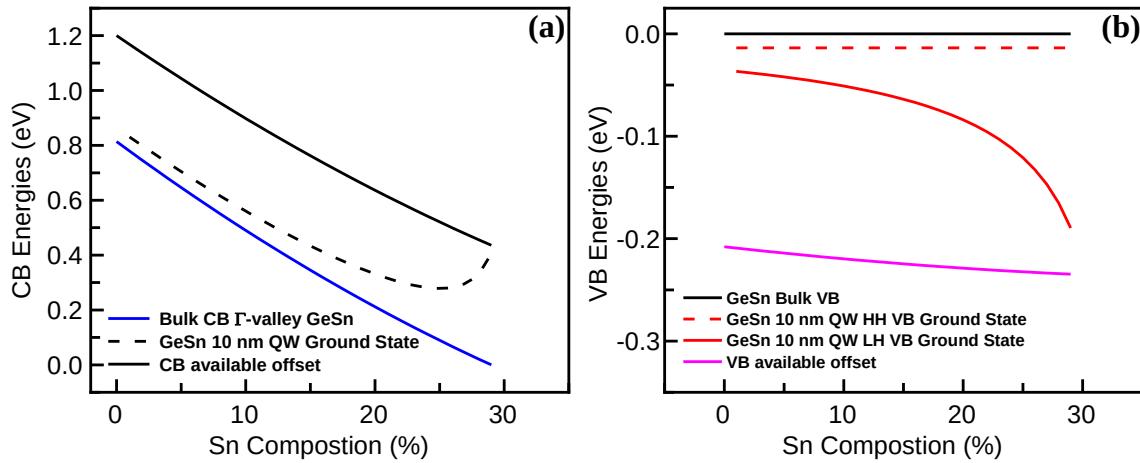


Figure 98. Band-offsets and ground state eigen energies as a function of Sn composition for (a) the CB and (b) VB in the 10 nm GeSn QW with a LM InGaAs QW barrier.

the VBO and consequently the CBO. This VBO for the Ge/GaAs (*i.e.*, the $\text{Ge}_{1-y}\text{Sn}_y/\text{In}_x\text{Ga}_{1-x}\text{As}$ QW system for Sn = 0 %) has been determined to be nearly $0.35 \times \Delta E_g$, consequently, this is used as an assumption to determine the offsets for the $\text{Ge}_{1-y}\text{Sn}_y/\text{In}_x\text{Ga}_{1-x}\text{As}$ QW system as the compositions are changed. Note that the total offset is also summarized in **Figure 95(c)**. Based on these estimates, it is possible to determine if the carriers in the CB and VB will be confined in the QW even at room temperature. Note that due to the finite band offsets for the GeSn QW, the eigen energies as well as the electron and hole wavefunctions are calculated considering their offset dependence. The ground state eigen energies in the Γ -valley and the CBO are shown in **Figure 98(a)** and the electrons in the Γ -valley would be confined for most of the Sn compositions. Similarly, the holes in the VB are confined in the HH-band, and the corresponding ground state eigen energies and band offset available are shown in **Figure 98(b)**. At higher Sn compositions due to the rising quantum confinement effect (QC) associated with the reduced effective mass of GeSn, the carriers are more likely to escape. Carrier confinement for the holes in the HH-band is

not affected by the Sn alloying effect as the effective mass of the HH-band holes is large and doesn't change significantly, unlike the electrons in the Γ -valley and holes in the LH-band.

An interdependent relationship exists between the impact of Sn alloying and the effect of quantization on the lasing operation of the $\text{Ge}_{1-y}\text{Sn}_y$ QW laser. It is interesting to note that due to the quantization of the energy levels in the $\text{Ge}_{1-y}\text{Sn}_y$ QW, the bandgap is not zero even at Sn = 25 %, contrary to the bulk $\text{Ge}_{1-y}\text{Sn}_y$ bandgap [27, 28]. This creates an exciting regime where the transition energy for the active region is largely determined by the quantization effect, with no or minimal contribution from the bulk bandgap. Increasing the Sn composition has the following effects on the $\text{Ge}_{1-y}\text{Sn}_y$ active region: (i) decreasing the effective mass of the Γ -valley [31], (ii) decreasing the effective mass of the LH-band [31] and (iii) lowering the Γ -valley. The decreasing effective mass results in a drastically large QC pushing the ground state eigen energy higher and consequently, the effective bandgap rises. Whereas, increasing Sn composition also decreases the bulk bandgap of $\text{Ge}_{1-y}\text{Sn}_y$ material. Thus, these two effects cause opposing impacts on the $\text{Ge}_{1-y}\text{Sn}_y$ emission characteristics. The rising ground state eigen energy at higher Sn compositions (a consequence of the lower effective mass) is shown in **Figure 98**. A larger Sn composition produces a larger QC and Sn alloying impact on the lasing performance of the $\text{Ge}_{1-y}\text{Sn}_y$ QW laser. Thus, designing a $\text{Ge}_{1-y}\text{Sn}_y$ QW laser must include consideration of the Sn alloying effect on the bandgap as well as the Sn alloying effect on the effective mass and corresponding QC.

7.6 GeSn SCH QW Gain spectra and maximum net gain

The emission characteristics of the proposed $\text{Ge}_{1-y}\text{Sn}_y$ SCH QW structure can be estimated through knowledge of the band properties. Through 30×30 **k.p** calculations [31], the band energies, effective masses, and composition dependence of various conduction bands (CBs) and valence bands (VBs) in $\text{Ge}_{1-y}\text{Sn}_y$ alloys are predicted [31]. The refractive index and band energies for $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Al}_{1-x}\text{As}$ are adopted from Ref. 32. The 3-slab waveguide model was used to calculate the optical confinement in the $\text{Ge}_{1-y}\text{Sn}_y$ QW. The gain spectrum and threshold characteristics for the GeSn QW are calculated using a custom in-house gain solver [6, 15, 16] fed with 3D electrical profiles calculated through calibrated models via Sentaurus TCAD [33]. The simulation model includes the structure shown in **Figure 93(a)**. This includes the barriers around the GeSn QW formed by InGaAs and InAlAs cladding layers confining the optical E-field through a large refractive index difference. Critical material properties are considered for each material utilizing a dense numerical meshing in the model. There is added confidence in the electrical profiles in the system as the material properties used for all III-V materials and Ge are physically detailed and well-calibrated by Synopsys Sentaurus TCAD [33] over the years and for Ge and InGaAs nanoscale-electrical device simulations [2, 3], also discussed in previous Chapters. These models include a vast range of ideal and non-ideal physical phenomena such as multivalley band structure, MLDA, drift-diffusion, density gradient, various mole fractions, mobility and doping dependencies, *etc.* The electrical probes/contact are connected to the outermost layers, *i.e.*, the highly doped n and p regions so that electrical injection can spread into the entire laser stack, similar to where one would connect probes on a physically fabricated laser device. Along with the impact of the GeSn active region material properties, the results shown here include a large impact on the composition, mobility, band structure, thickness, conductivity, hetero-transport, refractive index, and doping of the III-V layers in the laser stack.

The material gain spectrum for the TE and TM mode emissions from the GeSn/InGaAs LM QW laser stack is shown in **Figure 99(a)** and **(b)**, respectively. Only the fundamental TE and TM modes are considered in the calculation for simplicity, in practice a quasi-TE and/or quasi-TM emission is expected as discussed earlier. Emissions are possible through the Γ -HH transition as well as Γ -LH transition [15, 16], and the relevant transitions in the energy range from 0.2 eV to 1 eV are considered and computed according to Fermi's Golden Rule [15, 16]. The TE mode gain

dominates over the TM mode gain as the TE mode gain is produced mainly from the HH-band which has a higher DOS [6, 15]. The ground state transition Γ -HH is denoted by the “B” peaks shown in **Figure 99(a)**, and as the Sn composition is increased, the peak moves to a lower energy. Transitions from the LH band also contribute to the TE gain, but at a slightly higher emission

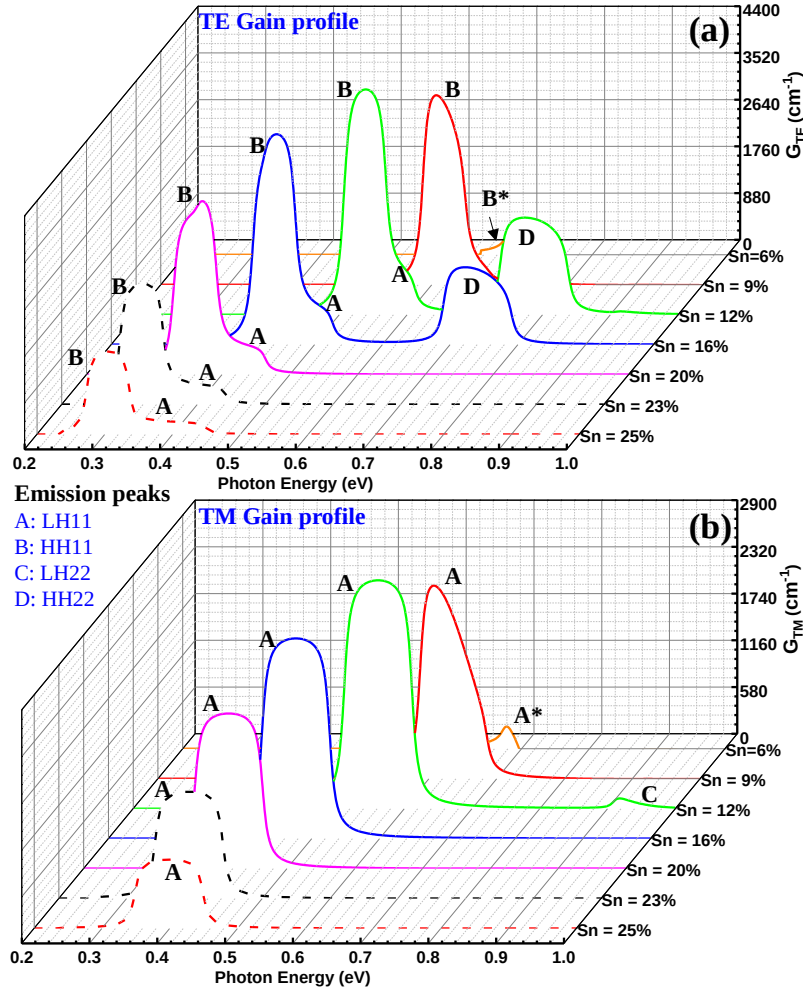


Figure 99. Material Gain spectrum for a 10 nm GeSn QW for various Sn compositions at a maximum carrier injection level of $\sim 10^{13} \text{ cm}^{-2}$: (a) TE mode gain and (b) TM mode gain. (*) a higher injection level compared to others is used to get some gain due to the insulating nature of the stack.

energy due to the quantization-induced broken degeneracy of the LH and HH bands. These ground state Γ -LH transitions denoted by the peak labeled “A” are shown in **Figure 99(a)**. Emission from the second order transitions are possible at higher emission energies and higher excitation levels, and the peaks associated with the first excited state Γ -HH transition are shown in **Figure 99(a)** labeled as “D”. Similarly, the TM mode gain is computed and shown in **Figure 99(b)**. The TM gain originates primarily from the ground state and excited state of the Γ -LH transitions [6, 15].

Note that a minute TE and TM gain peak is observed for the 6 % GeSn QW laser configurations in **Figure 99(a)** and **(b)**, respectively. For low Sn compositions, due to the poor conductivity of the surrounding InAlAs layers (very low In %), a sufficient quasi-fermi-level separation for the GeSn/InGaAs/InAlAs laser stack cannot be achieved for realistic injection levels. Hence, the proposed GeSn/InGaAs/InAlAs SCH QW laser stack cannot function as an efficient laser at Sn compositions below 7 %, as is evident from the maximum gain shown in **Figure 99**.

The maximum material and modal gain for the TE and TM modes are shown in **Figure 100(a)**. At the electrical probes (outside the n and p regions), the bias is increased resulting in a modulation of the fermi levels in the hetero-stack and a corresponding increase in separation of the quasi-fermi levels in GeSn QW and a rise in injection carrier density. The gain nearly saturates at higher injection levels, this can be seen in **Figure 100(a)**, as well as in typical III-V lasers such as in Ref. [34]. This saturation value is the maximum gain shown here in **Figure 100**. There exists an optimum range of Sn compositions between 8 - 18 %, where this GeSn QW laser stack can provide excellent material gain at realistic injection levels. At low Sn compositions below 7 %, the material gain is low due to the poor fermi-level modulation associated with the low conductivity high bandgap InAlAs layers in the stack as well as the poor directness of GeSn. As the Sn composition is increased, the DOS effective mass of the Γ -valley electrons reduces, while also reducing the joint-DOS in a nearly linear fashion and consequently reducing the gain factor [31]. According to Fermi's Golden rule, the transition rate for a constant photon density depends inversely on the transition energy [16], indicating that transitions that have a smaller energy difference would be more likely and will produce greater gain. Expectedly, as the Sn composition in the GeSn QW is increased, the effective transition energy reduces, increasing the transition rate as well as the gain factor. The momentum matrix element that determines the polarization-specific transition strength also depends on the effective mass and the transition energies, thus affecting the Sn composition dependence of the gain in more subtle ways. Due to the opposing effect of the transition rate (increasing) and DOS (reducing) on the Sn-composition dependence of the material gain, there exists a brief range of Sn compositions between 8 - 18 % where the gain factor increases or remains nearly constant even though the DOS drops linearly. The maximum gain is further scaled by the fermi factor which generates the material gain seen in **Figure 100(a)**. More details of the material gain calculation, transition rates, and band energies are provided in Chapter 5. Beyond a Sn composition of 16 – 18 %, the DOS reduction (due to reducing effective mass)

dominates, resulting in a drastic drop in material gain. Finally, the dependence of the maximum material gain (see, **Figure 100a**) on the Sn composition in the GeSn QW can be understood through 3 regions: (i) at low Sn compositions below 7 %, the gain factor is large and nearly constant but the fermi level modulation is not possible due to the AlAs in the SCH resulting in low gain, (ii) at Sn compositions between 8 – 18 %, the gain factor approaches a maximum value and remains nearly constant while the InAlAs SCH allows fermi level modulation and population inversion resulting in a maxima for the gain, and (iii) beyond ~ 18 %, the gain factor drops drastically due to low DOS resulting in a poor gain further degraded by the large separation between the bandgap and the effective bandgap due to QC. The modal gain is obtained by accounting for the confinement factor (**Figure 96b** and **c**) for the GeSn QW and is shown in **Figure 100(a)**. It follows a similar trend to the material gain and a peak modal gain value of $\sim 60 \text{ cm}^{-1}$ can be attained near Sn ~ 14 % for an emission wavelength of $2.6 \mu\text{m}$.

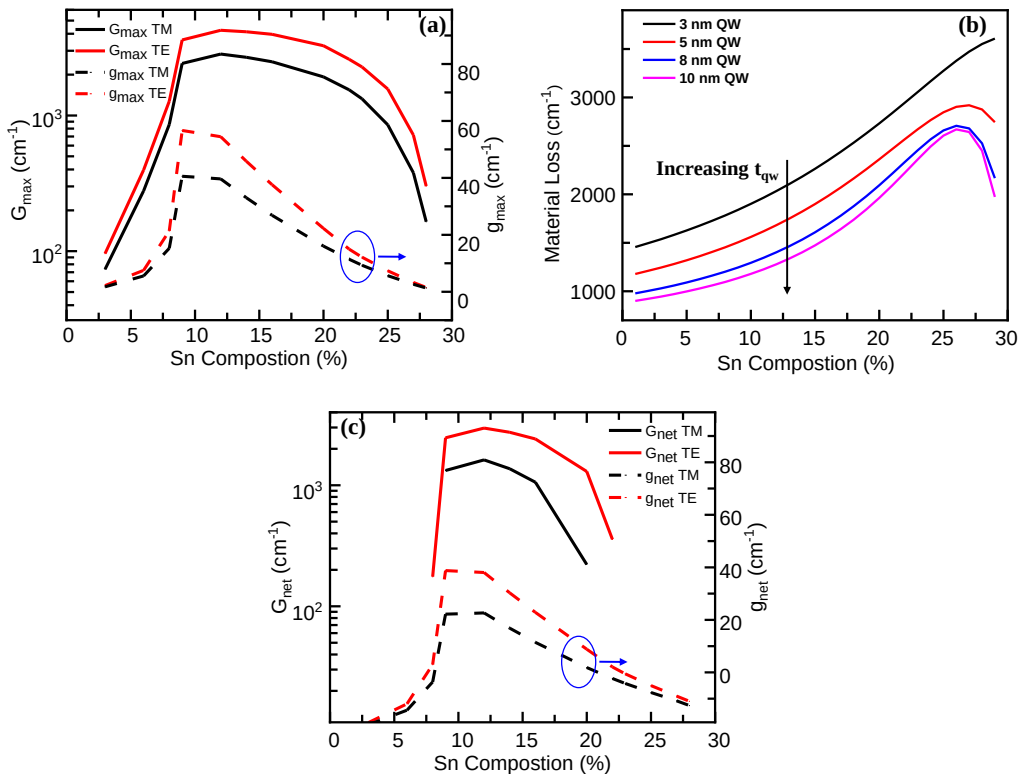


Figure 100. Lasing performance of the 10 nm GeSn QW as a function of Sn composition: (a) The maximum material and modal gain at a maximum carrier injection level of $\sim 10^{13} \text{ cm}^{-2}$, (b) the loss associated with the laser cavity for various quantum well thicknesses, and (c) the net material and modal gain potentially achievable beyond losses at a maximum carrier injection level of $\sim 10^{13} \text{ cm}^{-2}$.

As the QW thickness is increased, a larger optical confinement factor can be attained due to a larger overlap with the emission field [6, 15]. On the other hand, as the Sn composition is increased, the emission wavelength increases, and the optical confinement factor reduces. These trends of the optical confinement factor are summarized in **Figure 96(b)** and **(c)** also affect the cavity losses as shown in **Figure 100(b)** [6]. These losses are calculated assuming a free carrier absorption of 500 cm^{-1} and a mirror loss of 10 cm^{-1} , similar to the GeSn values reported in Ref. 11. Based on the material gain and loss, the net material and modal gain (*gain - loss*) are determined as shown in **Figure 100(c)**. Eventually, at Sn $\sim 22 \%$ the net modal gain becomes < 0 indicating no net lasing. A significant TE net modal gain of $\sim 40 \text{ cm}^{-1}$ can be attained at Sn $\sim 14 \%$ for the GeSn proposed QW laser structure. Net material and modal gains approaching $\sim 3000 \text{ cm}^{-1}$ and 40 cm^{-1} indicate that the proposed GeSn QW laser stack is an interesting avenue to explore lasing from this material system.

7.7 GeSn SCH QW system: Lasing Threshold

Sn alloying in GeSn produces a downward shift in the Γ -valley and has a low impact on the L-valley, unlike the tensile Ge QW case where the L-valley also descends with a certain rate [6]. This proves to be a significant advantage for the injection performance of the GeSn QW-based laser because, with rising Sn composition, the probability of occupation of the L-valley decreases much faster. Carriers in the L-valley do not participate in optical transitions due to the indirect nature of the transition, resulting in loss of carriers, high J_{TH} , and poor IQE. As the L-valley has a large DOS, de-populating this valley is critical and non-trivial, alloying with Sn greatly reduces its occupancy enabling the GeSn QW laser to have low J_{TH} . Furthermore, as seen earlier, the joint-DOS reduces linearly with increasing Sn composition due to the effective mass. A smaller DOS in

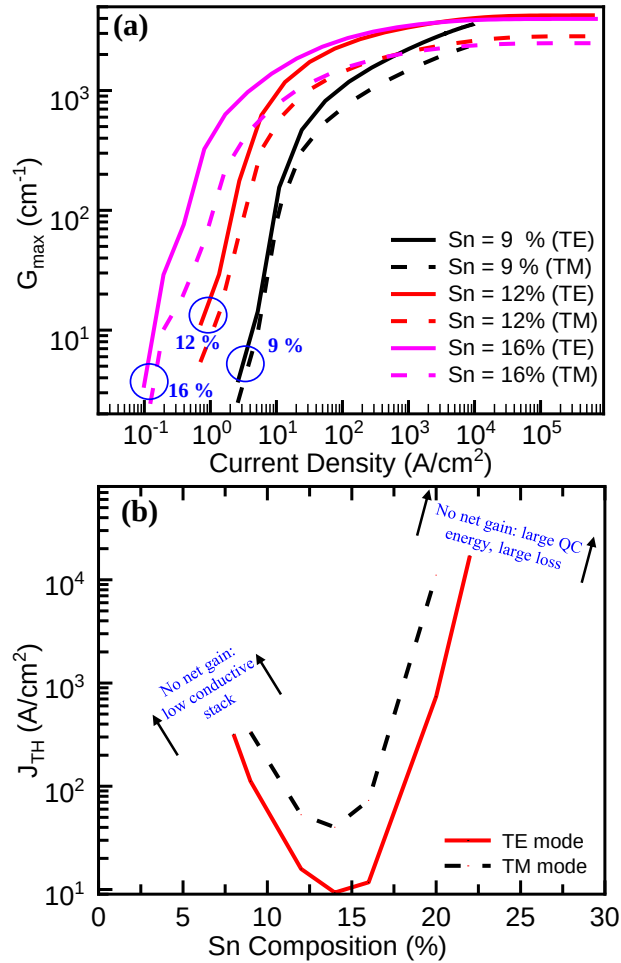


Figure 101. (a) Material Gain as a function of current injection. (b) Threshold current density required to overcome losses as a function of Sn composition in a 10 nm GeSn QW laser stack.

the QW enables transparency to be achieved at lower injection levels enabling a low J_{TH} provided there is some net gain. The J_{TH} is determined by the transparency injection level as well as the loss in the waveguide. Between 8 – 18 % Sn composition, the joint-DOS decreases linearly, but the material gain and the net gain remain high and non-decreasing (see, **Figure 100**). Hence, we can expect the GeSn QW laser to provide drastically low J_{TH} with a good net gain.

The current injection performance of the GeSn QW laser structure is summarized for Sn = 9, 12, and 16 % in **Figure 101(a)**. The gain characteristics move to lower current levels as the Sn composition is increased indicating that the transparency in the GeSn active layer is achieved at lower injection levels. Based on the total losses shown in **Figure 100(b)** and the material gain injection profile shown in **Figure 101(a)**, the J_{TH} can be determined as the injection current required to overcome the losses. This J_{TH} is shown in **Figure 101(b)** and an inflection point can be observed near Sn = 14 %, where the J_{TH} is the lowest. At large Sn compositions beyond ~ 20 %, the J_{TH} is large due to the high loss associated with the poor optical confinement as well as the reduced net gain. At low Sn compositions below Sn ~ 7 %, the J_{TH} is large due to the poor injection capability of the laser stack resulting in low fermi-level modulation, and low gain in the QW. At Sn ~ 14 %, the J_{TH} as low as ~ 10 A/cm² can be achieved for the TE mode owing to the cumulative additive effect of (i) QW configuration, (ii) large energy separation between the Γ - and L- valleys, (iii) strongly direct bandgap nature of GeSn at Sn = 14 %, (iv) low bandgap of GeSn, (v) sufficient band offsets, (vi) low joint-DOS, (vii) SCH optical confinement, (viii) low absorption losses, (ix) non-decreasing and high gain between Sn ~ 8 - 18 % although DOS decreases, and (x) reduced non-radiative recombination rates justified by the virtually defect-free LM interfaces.

7.8 Future outlook: Tensile GeSn and MQW

An interesting avenue for the proposed lattice-matched system is utilizing the growth ease associated with the LM to form a GeSn-on-InGaAs-on-InAlAs MQW SCH laser structure with type I alignment. Such a system would provide similar advantages to the GaAs-AlGaAs material system which revolutionized semiconductor lasers over the last half century [15, 17, 35]. Although such a GeSn-InGaAs MQW material system has not been reported yet, it shows great promise due to the possibility of large gain, lower J_{TH} , low defects due to the LM, direct bandgap nature of GeSn and III-V epi-growth know-how as well as the accelerating GeSn popularity. Moving to a GeSn MQW system from a SQW laser stack, certain physical phenomena need to be considered. Here, we list and qualitatively discuss some of these effects. Certain defects and dislocations may be present in any real heteroepitaxial system, and a detailed characterization of these issues can help quantify and understand the impact of the defects. However, a lattice-matched system is the best-known method to have the least defects in heteroepitaxial multilayer systems. In MQW systems, these potential defects may interact with each QW differently creating an unwanted impact on the gain, confinement, band alignment, offsets, and the injection into each QW. This can result in noise, reliability, and loss in lasing performance metrics such as gain and IQE. Additionally, incomplete relaxation of the underlying LGB can result in residual strain in the active region which can relax and create defects in the QW regions which are inherently unpredictable. This can again adversely affect the lasing metrics such as IQE and loss.

The confinement factor is expected to increase with an increase in the number of QWs due to a larger overlap with the optical field and a larger emitting volume [15, 17]. There is an initial increase due to a larger geometrical overlap, this eventually saturates [15, 35]. There will be an optimum number of QWs for maximum confinement factor and this will depend on the wavelength, QW thickness, composition, and SCH waveguide stack [35]. Beyond this optimum number, the J_{TH} will rise significantly without providing a gain benefit. Each QW active region will not overlap the same with the optical field, so the contribution of gain from each QW will be different. For a symmetric design, the central QW could be aligned perfectly with the E-field peak resulting in a maximum contribution to the confinement factor and the gain. The QWs toward the edges will have a smaller E-field overlap resulting in a smaller confinement factor and a smaller gain. For every additional GeSn QW, a non-emitting InGaAs QW barrier is also added, and since

the confinement factor has a large geometrical dependence, these increasing barrier layers result in reducing confinement factor.

The modal gain is expected to rise linearly with the number of QWs following the confinement factor trend (material gain remains nearly independent of the number of QWs). The threshold current density (and J_{MAX}) will increase linearly with the number of QWs due to a larger number of carriers that are now required in the active regions, owing to the increased volume of the active region. Although many QWs can provide a large gain, this comes at the cost of higher current consumption through the J_{TH} [36] and J_{MAX} . IQE is an intrinsic material property dependent on the band structure of GeSn QW and defects and various transitions in the active QW, it would not be affected by many QWs. Considering these factors, certain ideal-case estimates can be predicted for a 3 QW GeSn-InGaAs lattice-matched laser. The Sn and In composition can be assumed to be 15 % and 30 %, respectively, resulting in an emission of 2.7 μm . Upon optimizing the waveguide cavity based on the adaptive design, one can expect an optical confinement factor of nearly 3 % ($\sim 3\times$ with respect to **Figure 96b**) and material gain of $\sim 4000\text{ cm}^{-1}$ (see **Figure 100a**) with a material loss of $\sim 1500\text{ cm}^{-1}$ (see **Figure 100b**). The net modal gain in this 3 QW system can be estimated to be 75 cm^{-1} with a J_{TH} of $\sim 30\text{ A/cm}^2$.

Considering the growing number of investigations in achieving lasing and improving the lasing performance of Ge, SiGeSn, and GeSn-based light sources, additional design flexibility for future modifications could be beneficial. Although the $\text{Ge}_{1-y}\text{Sn}_y$ QW design proposed here is a fully lattice-matched system, various reports have studied light emission from Ge-based sources (theory as well as experiment) using epitaxial compressive [11] and tensile strain [4, 6, 35]. A detailed report on tensile strained Ge QW laser and lasing from Ge (and GeSn) based systems is summarized in Ref. 6. As the explorative efforts for GeSn lasers are still in the early stages of investigations, compressive strain in GeSn is also being investigated on Si or GaAs systems [12, 37 - 39]. Considering this evolving research area, compressive and tensile strain in $\text{Ge}_{1-y}\text{Sn}_y$ could prove to be technologically feasible as well as provide performance benefits. The $\text{Ge}_{1-y}\text{Sn}_y/\text{In}_x\text{Ga}_{1-x}\text{As}$ SCH QW structure can be used to introduce a small mismatch, either compressive or tensile by changing the InAs composition in the structure away from LM. Such a system could be used to tune the lasing performance of single QWs, MQWs, and, strain-balanced structures by creating tensile or compressive GeSn active layers. The InAs composition in InGaAs required to create a small tensile strain of 1 % (t1), 2 % (t2) as well as a small compressive strain of 1 % (c1) and 2 %

(c2) is shown with respect to the LM case, shown in **Figure 102**, where InAs compositions for each compressive and tensile strained are indicated in this figure. A potentially additive effect of tensile strain and Sn alloying in the GeSn active layer could enable efficient lasing from group-IV-based materials. Furthermore, in the large-scale growth of these GeSn-InGaAs-InAlAs SCH structures, the LGB relaxation and design are crucial and challenging as pointed out earlier. Using the InAs composition as a tuning mechanism following **Figure 102**, designers can offset unwanted strain in the LGB or material stack to ensure desired LM properties in the active region.

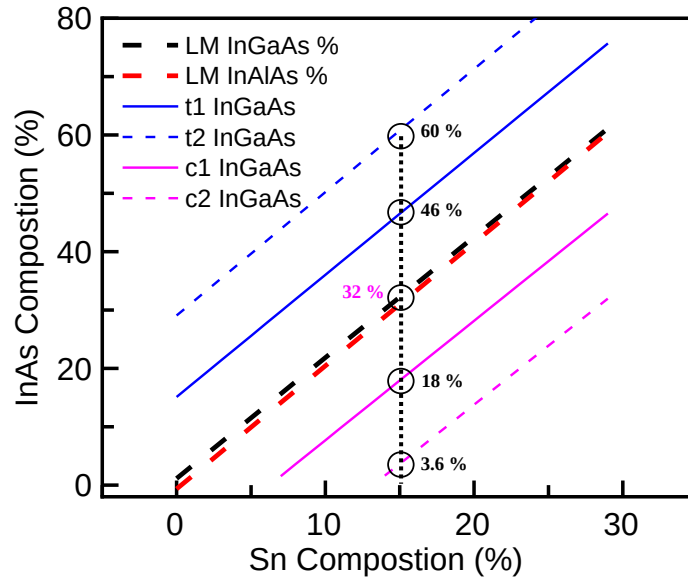


Figure 102. An extension beyond LM GeSn QW: The proposed GeSn SCH QW system can also leverage the potential benefits of a small tensile or compressive epitaxial strain provided the benefits of strain outweigh the benefits of LM.

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Concluding Remarks

Can Germanium become a Beyond Moore solution for extending the transistor roadmap beyond traditional Si devices? Can Ge and GeSn form quantum wells for efficient lasing in the MIR spectral range? Through this work, these two broad questions are addressed along with numerical and experimental explorations. This work discussed how good quality Ge and GeSn thin films can be grown using MBE via III-V buffers, characterized and modeled to predict transistor and QW laser operability as well as metrics. The key contributions of this work can be summarized as follows:

1. Alternate channel CMOS material-to-device-to-circuit co-optimization for a tensile Ge on InGaAs based FinFET system. This monolithic system operated at 0.5 V supply while providing a high electron mobility InGaAs n-channel as well as a high hole mobility Ge p-channel. The extensive tunability and design considerations of this system by varying the tensile strain through the In composition are presented.
2. Ge grown lattice-matched on AlAs can form multi-layer structures suitable for advanced Angstrom era high mobility NSFETs. The AlAs can act as a sacrificial layer during the process, resulting in superior etch selectivity compared to existing processes while acting like a conduction barrier. The process variation immunity is seen to be a huge advantage for yield and reliability. The LM Ge layers can be defect-free resulting in reliable operation and high yield. The material-to-device-to-circuit co-optimization for this monolithic LM system is discussed while evaluating the performance at advanced nodes.
3. A Ge-based Quantum well laser is introduced which uses the underlying InGaAs layer as a strain template and QW barrier as well as the waveguide. The performance of such a monolithic laser is seen to be orders of magnitude better in terms of threshold current density, IQE, and net gain, compared to previous Ge laser reports. Through experiments, the band alignment and minority carrier lifetime is determined for

multiple samples and fed to the numerical solvers. A detailed theoretical framework specific to tunable tensile Ge lasers and waveguides is built and metrics are evaluated.

4. The optical constants n (refractive index), k (extinction coefficient) and absorption coefficient as well as the dielectric constants such as ϵ_1 and ϵ_2 are evaluated for multiple tensile strained Ge samples grown on a composition-controlled InGaAs LGB and InGaAs strain template. The samples are grown using MBE and analyzed using VASE. An interesting physical phenomenon associated with the movement of the band structure with tensile strain was discovered through the critical point analysis and fitting. This is the first report of impact of tensile strain on dielectric and optical constants of epitaxial thin film Ge, this can enable better design and analysis of optoelectronic devices based on Ge.
5. Alloying Ge with small percentages of Sn can enable better optical emission from GeSn. A new monolithic system where the entire SCH QW laser structure utilizing GeSn-InGaAs-InAlAs can be formed by lattice matching all the layers. This LM system can have benefits similar to the GaAs-AlAs laser system, and some of the performance metrics such as gain spectrum, threshold current and net gain are presented. Ultra-low threshold current density is possible at $\sim 14\%$ Sn composition with a good operation range between 8-18% Sn. The wide applicability and efficient lasing operation is presented.

Future Outlook

The discussion and results in this work can motivate research endeavors relating to tensile and lattice matched Ge grown epitaxially on III-V layers. Explorations with device fabrication, advanced simulation and characterization can provide better insights into many applications. Relating to the **tensile strained Ge on InGaAs** systems,

1. Experiments to find the critical layer thickness of Ge as function of biaxial tensile strained Ge. Such a study will require multiple sample growths and characterization, but convey an important understanding similar to what exists for compressive systems.
2. Fabrication of a co-integrated long channel CMOS inverter, utilizing high electron and hole mobility channels to validate some of the predictions in this work.
3. Using optical excitation, the transition point where the TM gain begins to dominate over the TE gain in the tensile Ge QW laser can be determined.
4. Static and Dynamic analysis of tensile Ge laser in a single and multiple quantum well configuration.

Relating to the **LM Ge on AlAs** systems,

1. An important extension of the NSFET design is the CFET set to arrive in 2034 in the IRDS. The Ge-AlAs system can form process immune high performance CFET standard cells such as NAND and NOR. This would be the path to universal logic based on Ge CFETs.

Relating to the **LM GeSn on InGaAs** systems,

1. Static and Dynamic analysis of LM GeSn laser in a single and multiple quantum well configuration can provide insights into the operation as a product.
2. Growth and fabrication of a moderate Sn composition LM SCH QW stack (GeSn-InGaAs-InAlAs) and consequent stripe laser fabrication.

Of course, many more exploration are possible to build and improve upon the analysis presented in this work. This was a list of some of them.

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