



Silicon Compatible Electrically Pumped Direct Bandgap Ge/GeSn Laser

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11/18/2019
Final Report

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REPORT DOCUMENTATION PAGE					<i>Form Approved</i> OMB No. 0704-0188	
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1. REPORT DATE (DD-MM-YYYY) 08-06-2020		2. REPORT TYPE Final Performance		3. DATES COVERED (From - To) 30 Sep 2015 to 29 Sep 2019		
4. TITLE AND SUBTITLE Silicon Compatible Electrically Pumped Direct Bandgap Ge/GeSn Laser				5a. CONTRACT NUMBER		
				5b. GRANT NUMBER FA9550-15-1-0388		
				5c. PROGRAM ELEMENT NUMBER 61102F		
6. AUTHOR(S) Jelena Vuckovic, Krishna Saraswat				5d. PROJECT NUMBER		
				5e. TASK NUMBER		
				5f. WORK UNIT NUMBER		
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) LELAND STANFORD JUNIOR UNIVERSITY 450 SERRA MALL STANFORD, CA 94305-2004 US				8. PERFORMING ORGANIZATION REPORT NUMBER		
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) AF Office of Scientific Research 875 N. Randolph St. Room 3112 Arlington, VA 22203				10. SPONSOR/MONITOR'S ACRONYM(S) AFRL/AFOSR RTB1		
				11. SPONSOR/MONITOR'S REPORT NUMBER(S) AFRL-AFOSR-VA-TR-2020-0050		
12. DISTRIBUTION/AVAILABILITY STATEMENT A DISTRIBUTION UNLIMITED: PB Public Release						
13. SUPPLEMENTARY NOTES						
14. ABSTRACT We have made several important contributions towards implementation of a practical CMOS compatible laser, including: 1. A rigorous analysis of the strong interaction between uniaxial strain and parasitic absorption in germanium with major implications for Si-compatible lasing 2. Experimental demonstration of a strained Ge light source 3. Silicon-Compatible Fabrication of Inverse Woodpile Photonic Crystals with a Complete Band Gap						
15. SUBJECT TERMS silicon photonics, silicon based laser, electrically injected germanium based laser, optical interconnects						
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT UU	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON POMRENKE, GERNOT	
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NUMBER (Include area code) 703-696-8426	

Si Compatible Electrically Pumped Direct Bandgap Ge/GeSn 1 **Laser**

Grant: FA9550-15-1-0388
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Annual Report, Sept. 9, 2019

Abstract

CMOS compatible on-chip light source is the holy grail of silicon photonics and has the potential to alleviate the key scaling issues arising due to electrical interconnects. Despite several theoretical predictions, a sustainable, room temperature laser from group IV material is yet to be demonstrated. In this work, we show that a particular loss mechanism, known as inter-valence-band absorption (IVBA), has been inadequately modeled until now and that capturing its effect accurately as a function of strain is crucial to understanding light emission processes from uniaxially strained germanium (Ge). Apart from IVBA, other factors such as polarization, doping and carrier injection have been thoroughly accounted for using the first principle model and a complete roadmap towards a room temperature Ge laser is presented. Strikingly, a special resonance between gain and loss mechanisms at 4-5% uniaxial strain is found resulting in a high net-gain of more than 400cm^{-1} at room temperature. It is shown that achieving this resonance should be the goal of experimental work rather than pursuing a direct band-gap Ge.

Three-dimensional (3D) photonic crystals can provide access to very interesting and unique properties for ultimate control and manipulation of photons, not possible otherwise. However, widespread implementation of such photonic crystals remains elusive because the fabrication technology available today has either silicon (Si) incompatibility, poor scalability, a large number of undesired defects, challenging or impossible placement of intentional defects, or has advanced non-standard process steps available only in a few laboratories. In this work, a new methodology of fabricating defect-free 3D photonic crystals is developed which is ‘truly’ Si-compatible and uses techniques available in any standard fabrication facility. Using this methodology, a broadband omnidirectional reflector on Si is demonstrated. Introduction of intentional defect sites for fabrication of 3D waveguides and optical cavities is also discussed.

1. A rigorous analysis of the strong interaction between uniaxial strain and parasitic absorption in germanium with major implications for Si-compatible lasing

1.1 INTRODUCTION

Silicon photonics (SiPh) is considered a key enabling technology for future CMOS systems since it has the potential to alleviate the bandwidth-power-density bottleneck of electrical interconnects [1]. However, aggressive energy targets for interconnects have to be met before the technology can become the mainstream replacement for their electrical counterparts and therefore a fully integrated platform for SiPh is a necessity [1,2]. A CMOS compatible light source is the only missing piece in the otherwise well integrated SiPh technology [1,2]. Several approaches such as doping, strain and tin (Sn) alloying have been proposed [3-10] for lasing from germanium (Ge)

but a successful demonstration at room temperature is yet to be seen. Strain coupled with appropriate doping is a promising approach because it reduces the energy gap difference between direct and indirect bands, thereby increasing the electron population in the direct Γ valley which consequently leads to significantly lowered thresholds for lasing [3-8]. However, the parasitic free carrier absorption (FCA) in the valence bands, also known as intervalence band absorption (IVBA) has been experimentally and theoretically shown to incur so significant a loss that it nullifies any material gain achieved through strain and/or doping [11-14]. Despite the fact that IVBA is a major barrier in the realization of a room temperature group IV light source, there has been no major study which accurately models it and systematically captures the effect of strain on this parasitic absorption. Most of the modeling work to date assumes a simple closed form expression for IVBA which was obtained by a sparse fit of the measured absorption in relaxed Ge as in Ref. [3] or on slightly strained (0.2%) Ge as in [4,11]. In this work, we instead model IVBA and the material gain of Ge under various amounts of uniaxial tensile strains using first principles. We show that the simple IVBA expression used in the bulk of published literature significantly deviates from the predictions of our rigorous model and that it does not capture the essential physics particularly at high strain values. Using our model, we predict that positive net-gain from Ge can be achieved at room temperature only within a small window with uniaxial tensile strain between 4 and 5%.

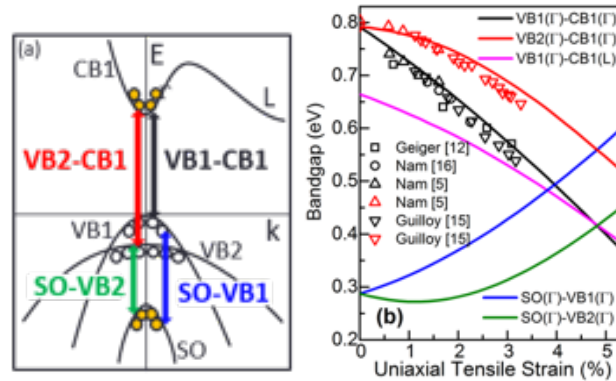


Fig 1(a) Schematic showing simplified band diagram of germanium and the main transitions in the light emission process, (b) Band-gap as a function of strain for the different transitions along with the available experimental data

Fig. 1(a) shows a schematic depicting the main band transitions involved in the process of light emission from Ge. The gain is mainly composed of direct transitions from the top two valence bands (VB1 and VB2) to the lowest conduction band (CB1) while the direct transitions from split-off band (SO) to VB1 and VB2 make up the majority of the IVBA loss mechanism [11]. Empirical Pseudopotential Method (EPM), discussed in Section II, is used to compute detailed band-structure of strained

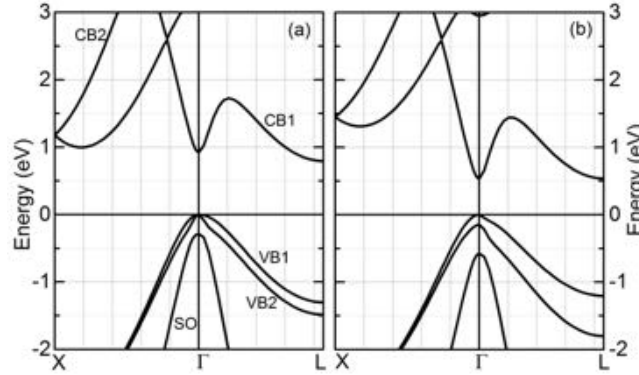


Fig 2 Band diagrams computed using the empirical pseudopotential method for uniaxial strain (a) 0% i.e. bulk Ge and (b) 5%

Table 1: EPM parameters used in this work

	Symbol	Unit	Value
Lattice constant	a	Å	5.658
Local form factor	V3	Ry	-0.236
	V8	Ry	0.019
	V11	Ry	0.056
Cubic spline interpolation slope parameters	S3	-	0.21
	S8	-	0.06
	S11	-	0.07
Pseudopotential cut-off parameters	a5	a.u.	4.5
	a6	a.u.	0.3
Spin-orbit parameters	zeta	Å ⁻¹	10.09
	mu	Ry	0.0017
Elastic Constants	C11	GPa	128.53
	C12	GPa	48.62

Ge (s-Ge) and the band-gap corresponding to all relevant transitions is shown in Fig. 1(b) along with the available experimental data. It is evident that the relative band-gaps corresponding to the transitions change significantly with strain and hence any expression derived for relaxed Ge may not capture the complete physics for highly s-Ge. For instance, consider the band-gap for VB1-CB1 (black curve in Fig. 1(b)) and for SO-VB1 (blue curve in Fig. 1(b)) transition. For bulk Ge, SO-VB1 band-gap is significantly smaller than VB1-CB1 and if the light emission occurs with photon energy approximately equal to VB1-CB1 band-gap, the probability that it will be absorbed by SO1-VB1 transition will be relatively small. However, the band-gaps for those two transitions become equal (black and blue lines intersect) around 4% uniaxial strain. At this point the photons emitted due to VB1-CB1 transition can be easily absorbed by the large number of allowed states corresponding to SO-VB1 transition. Section III will elaborate on this important resonance effect of strain on the gain and loss mechanisms. For s-Ge, the polarization of light becomes an important factor due to band-mixing effects in the valence band and the momentum matrix elements that capture the polarization effects need to be accurately accounted for. Section IV deals with understanding these momentum matrix elements and the crucial role they play in the light emission

process from s-Ge. Section V discusses the effect of carrier injection and doping and lays out a map depicting suitable conditions that will lead to lasing from s-Ge at room temperature.

1.2 SIMULATION METHODOLOGY AND COMPARISON WITH EXPERIMENTS

We have employed empirical pseudopotential method (EPM) for calculating the band structure of unstrained and s-Ge. EPM allows us to build scalable electronic models with relatively small number of empirical parameters required to obtain a given material's band structure. In the past, EPM has been used to describe the electronic properties of strained Si and Ge with remarkable success [17]. According to Chelikowsky and Cohen [18], the single electron Hamiltonian can be written as:

$$H(G, G') = -\frac{\hbar^2}{2m} \nabla^2 + V_{loc}(|G - G'|) + V_{nloc}(G, G') + V_{so}(G, G'),$$

where V_{loc} , V_{nloc} , and V_{so} represent the local, nonlocal, and spin orbit contributions to the pseudopotential, respectively. We have used a basis set $\{G\}$ consisting of 169 plane waves to expand the pseudopotential in the reciprocal space. V_{loc} depends only on the magnitude of the reciprocal lattice vector $q=|G-G_0|$ and V_{nloc} captures the angular momentum dependence of the pseudopotential. For obtaining band structure of pure unstrained material, the local pseudopotential form factors are required only at certain discrete values of reciprocal lattice vector given by $q^2 = \{0, 3, 8, 11\} * (2\pi/a_0)^2$. However, for band structure

calculation of s-Ge, local pseudopotential at an arbitrary reciprocal vector q is needed and is obtained by performing cubic spline interpolation between local pseudopotential form factors V_{loc} at discrete q values mentioned above [19]. For the interpolation, the slope of the curve at those discrete q points is used as a variable. The slope of the curve determines, among other properties, the change in band-gaps with strain (a.k.a. deformation potentials) and therefore, is a good choice to use as a parameter in the study of strained materials. Also, in order to ensure fast cut-off at large q^2 we have followed the approach of Ref. [20] and required:

$$V_{loc}(q) = V_{cubic}(q) \left(1/4 \tanh\left(\frac{a_5 - q^2}{a_6}\right) + 1/4 \right)$$

We use analytical expressions as in Ref. [19] for overlap integrals $B_{nl}(K)$ needed for evaluation of the matrix elements for spin orbit interaction:

$$B_{nl}(K) = \frac{5 - (K/\xi)^2}{5 \left(1 + (K/\xi)^2 \right)^4}$$

Table I lists the values of pseudopotential parameters used for Ge. The pseudopotential parameters for non-local corrections have been slightly modified from those in Refs. [17] and [18] so as to reproduce as closely as possible the band structure of Ge of Ref. [18]. Fig. 2(a) and 2(b) show the calculated band structure of relaxed Ge and Ge with 5% uniaxial strain, respectively. The variation of band-gap with strain is shown in Fig. 1(b) and the accurate matching of simulation data with different experiments proves its credibility. Table II compares the band-gaps and effective mass between the simulations and data from Ref. [21] and they both match exceedingly well.

Table 2: Band structure parameters compared with experiments

Band-gap	$\Gamma_v - \Gamma_c$	$\Gamma_v - L_c$	Δ_{so}	
This work	0.9214	0.7943	0.2871	
Literature	0.928	0.79	0.29	
Effective mass(e^-)	m_e^Γ	$m_{e,l}^L$	$m_{e,t}^L$	
This work	0.047	1.58	0.093	
Literature	0.049	1.568	0.094	
Effective mass(h^+)	m_{HH}^{100}	m_{HH}^{110}	m_{LH}^{100}	m_{LH}^{110}
This work	0.248	0.466	0.059	0.054
Literature	0.254	0.477	0.049	0.056

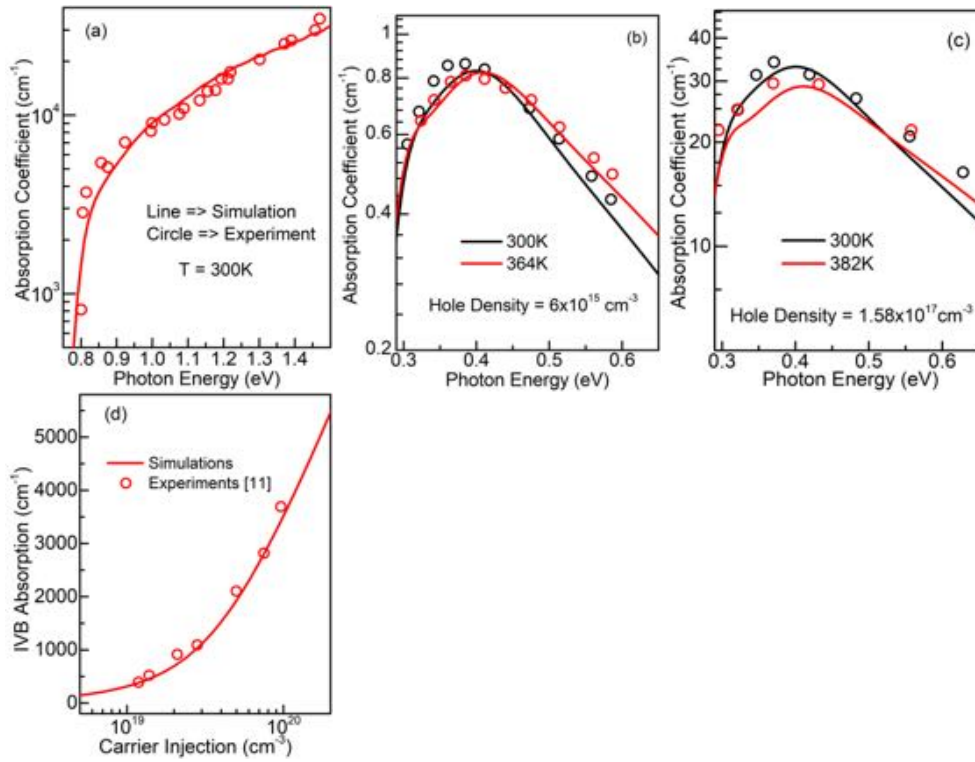


Fig. 3(a) Computed absorption spectrum of Ge matches well with the experiments [22] at 300K, (b) Infrared absorption of Ge due to IVBA compared with experiments from Ref. [23], (c) Infrared absorption of Ge for hole density of $1.58 \times 10^{17} \text{ cm}^{-3}$ is matched well with experiments from Ref. [24] and (d) IVBA as a function of carrier injection matches recent experiments from Ref. [11]

After calculating the band structures, Fermi's Golden Rule is used in order to calculate the transition rates between different bands in Ge. The absorption (or gain) due to band-to-band transitions is calculated using:

where, $C_0 = \pi e^2 / c n \epsilon_0 m_0^2 \omega$ is a constant.

The term $\delta(E_1(k) - E_2(k) - \hbar\omega)$ represents the joint density of states (JDoS) between bands 1 and 2 corresponding to direct transitions of energy $\hbar\omega$. It can be calculated directly from the band

structure of the material by counting the number of states between band 1 and 2 with an energy difference equal to $\hbar\omega$. $(f_1 - f_2)$ refers to the Fermi inversion factor. Each f_1 and f_2 are Fermi functions which depend on the band structure, doping and injection conditions in the material. The quantity $|\hat{e} \cdot \mathbf{p}_{12}(\mathbf{k})|^2$ is the momentum matrix elements for a particular wave vector $\mathbf{k}$ and $\hat{e}$ is the polarization. Momentum matrix elements p_{12} depend on wave function overlap between band 1 and 2. The wave functions for each band is obtained as a part of band structure calculations done using EPM. The three quantities – JDOS, Fermi inversion factor and momentum matrix elements are calculated at each point in the first Brillouin zone (FBZ) and their product is then summed throughout the FBZ to obtain the absorption (gain) spectrum. It should be noted that the only empiricism that enters the simulation methodology is through the pseudopotential of s-Ge. The rest of the methodology is based on first principles and there are no fitting parameters involved apart from the pseudopotential itself. Fig. 3(a) shows the absorption spectrum of bulk Ge at 300K. The simulation data matches the experimental data from Ref. [22] accurately. In this work, we have used the same formalism described above to calculate the IVBA as well. Fig. 3(b) shows the absorption spectrum of bulk Ge below its band-gap taken from experimental data in Ref [23]. This absorption is because of the IVBA transitions described before [11]. The simulation data matches accurately for a hole density of $6 \times 10^{15} \text{cm}^{-3}$ and two different temperatures. Different temperatures basically probe the correctness of Fermi functions used in the model and a good fit with experimental data proves the same. Fig. 3(c) compares the experimental data from Ref. [24] with simulations for a hole density of $1.58 \times 10^{17} \text{cm}^{-3}$. The simulations agrees with the experiments reasonably well. It was seen that the agreement between simulations and experiments became worse for higher hole densities in Ge. This can be explained by the fact that at higher doping levels the p-dopant atoms start to play a role in absorption [25]. However, in the case of s-Ge laser, holes are injected by means of optical or electrical excitation and not doping. As such, the effect of p-dopant atoms does not need to be accounted for. In order to remove the artifacts from dopant atoms, we compare the simulations with experiments in Ref. [11] where high concentration of holes in Ge was achieved by carrier injection instead of p-doping. Fig. 3(d) shows that the match between the two is exceptional. The good fit of absorption spectrum in Ge with experimental data taken from different sources under different operating conditions instils complete confidence in the model developed. This work is unique because we have used exactly the same basic formalism to describe all the transitions possible in this material system. Most of the other published work focuses on thorough formalism for gain but the loss mechanism such as IVBA is captured by means of an over-simplified expression fitted for bulk Ge. In the next section, we show that the over-simplified expression used in published work does not capture the complete physics and leaves out essential pieces that are crucial in understanding the process.

1.3 EFFECT OF STRAIN ON GAIN AND INTER VALENCE-BAND ABSORPTION

The formalism developed in the last section is used to study the effect of strain on gain and IVBA. Fig. 4 shows the band-to-band gain as a function of photon energy for different strain values in Ge. The band-to-band gain (denoted as just gain) is the sum of the gain obtained from transitions between VB1-CB1, VB2-CB1 and SO-CB1 bands. The gain curves are obtained for a doping of $2 \times 10^{19} \text{cm}^{-3}$ and a carrier injection level of $4 \times 10^{19} \text{cm}^{-3}$. The polarization of light is taken to be in a direction perpendicular to the strain axis. The effect of polarization, carrier injection and doping will be discussed in subsequent sections. Two important characteristics of the gain curve is that the peak gain increases with strain and it redshifts to lower photon energies. The peak gain

increases primarily because Ge becomes more direct with increasing strain i.e. the energy gap between L and Γ valley in CB1 reduces with strain. The peak gain redshifts because the band-gap of Ge (between VB1 and CB1) reduces with strain. These two characteristics are well established both theoretically and experimentally [3-13] and our simulation captures them accurately.

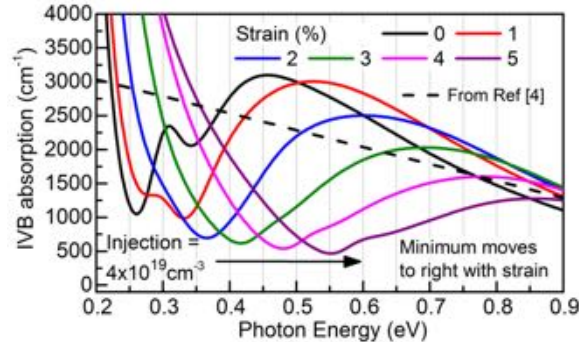


Fig. 4 Band to band gain as a function of photon energy and uniaxial strain. The doping and carrier injection is kept constant at $2 \times 10^{19} \text{cm}^{-3}$ and $4 \times 10^{19} \text{cm}^{-3}$ respectively.

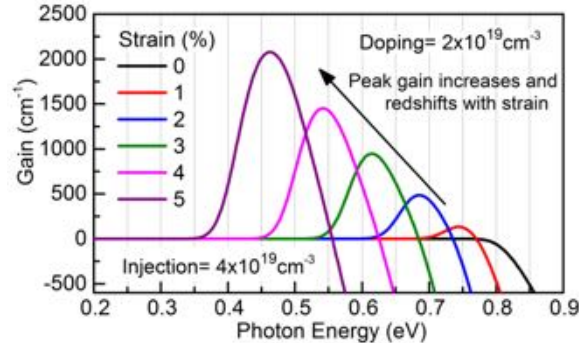


Fig 5: IVBA as a function of photon energy and uniaxial strain for a carrier injection level of $4 \times 10^{19} \text{cm}^{-3}$. The dashed line shows the IVBA used in prior literature and proves that it misses key features and becomes increasingly incorrect with strain

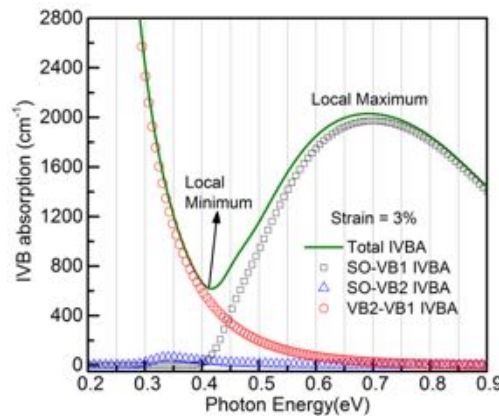


Fig. 6: The break-up of IVBA into different components shows that the SO-VB1 transitions plays the most important role in governing the location of maxima and minima

IVBA as a function of photon energy and strain is shown in Fig 5. IVBA is the sum of absorption due to transitions between SO-VB1, SO-VB2 and VB2-VB1. The curves are computed for the same strain values, doping, injection and polarization as was used for gain calculations in Fig. 4.

The dashed curve in the figure is the closed form expression of IVBA fitted for Ge with a small biaxial strain of 0.15% [4,11] and is widely used in literature to compute IVBA for different strain values in Ge and completely different operating conditions. It predicts a linear increase in IVBA with decreasing photon energy which is evidently not the case. As can be seen from the curves, there is a local maximum and a local minimum in IVBA and in order to understand these crucial extremes, Fig. 6 separates the different components of IVBA for 3% uniaxial strain. SO-VB1 dominates the IVBA with VB2-VB1 transition playing an important role at lower photon energies. SO VB2 transitions are limited because VB2 is mostly occupied at these injection levels making the number of allowed states for the transition very small. The local maximum corresponds to the increasing density of states (DoS) available for SO-VB1 transition limited by the Fermi function, which eventually dominates over increasing DoS and results in decaying IVBA beyond the maximum. The local minimum is because of lack of available states for transitions below SO-VB1 band-gap and limited by the allowed transitions between VB2 and VB1. Therefore, it is reasonable to conclude that the minimum in IVBA will occur at a photon energy which is approximately equal to the band-gap of SO-VB1 transition for a particular strain value. Since SO-VB1 band-gap increases significantly with strain (as shown in Fig. 1(b)), the minima in IVBA also shifts to higher photon energy with strain. As we apply strain to make the band-gap more direct, the Γ -VB1 separation shrinks and the SO-VB1 separation increases (shown in Fig. 1b). This red-shifts the emission wavelength below 0.8eV (Fig. 4) while simultaneously blue-shifting the parasitic IVBA curves (Fig. 5). Fig. 7 plots the gain (Fig. 7(a)) and IVBA (Fig. 7(b)) on the same energy scale to make it easily readable. It also shows the net-gain (Fig. 7(c)) obtained after subtracting IVBA from the gain.

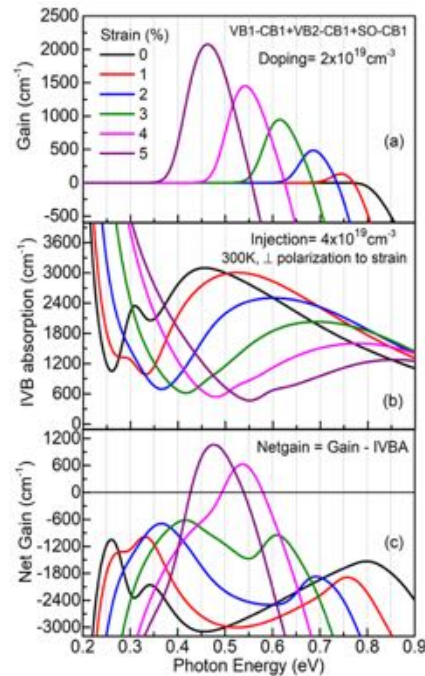


Fig. 7(a) Band to band gain as shown in Fig. 4 but at the same energy scale with IVBA in Fig. 7(b), 7(c) Net-gain obtained after subtracting IVBA in 7(b) from gain in 7(a)

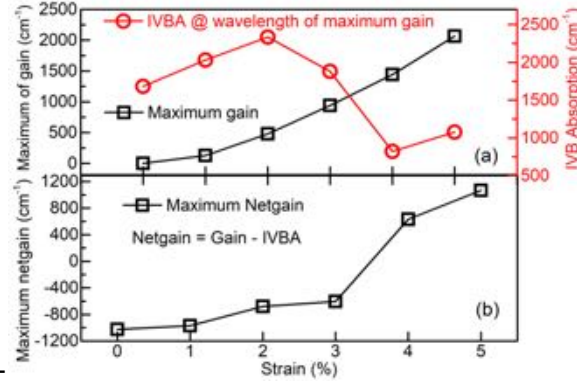


Fig 8(a) Maximum gain and IVBA at the wavelength of maximum gain extracted from Fig. 7, (b) Maximum net-gain extracted from Fig. 7(c)

With increasing strain, the maxima of the parasitic IVBA spectrum is brought closer to the emission wavelength up to 3% strain (green curves in Fig. 7) where the maximum in gain aligns with the IVBA maximum at 0.62 eV. Even more interestingly, further increasing the strain brings the emission wavelength out of alignment with the IVBA maximum and into alignment with the IVBA minimum, starting at 4% strain (pink curves in Fig. 7) where both the emission wavelength and IVBA minimum are close to 0.55 eV. This alignment remains until 5% strain beyond which IVBA increases rapidly due to VB2-VB1 transitions, thereby overwhelming any available gain. As a guide for the eye, we have extracted the maximum gain, IVBA at the wavelength of maximum gain and the resulting net-gain from Fig. 7 and plotted them in Fig. 8. It can be seen that strain initially worsens the IVBA, a large and hitherto ignored effect. Thus, increasing the strain from 0 to 3% results in a modest increase in net-gain, but further increasing the strain between 4 to 5% yields a dramatic increase in net-gain. This is a newly identified “resonance” effect and is shown explicitly in Fig. 7(c). The previous approach was a simple empirical fit that completely overlooked this very critical effect.

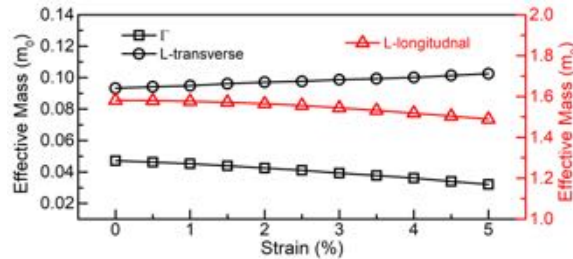


Fig. 9: Effective mass for the Γ valley and L valley do not change significantly with uniaxial strain

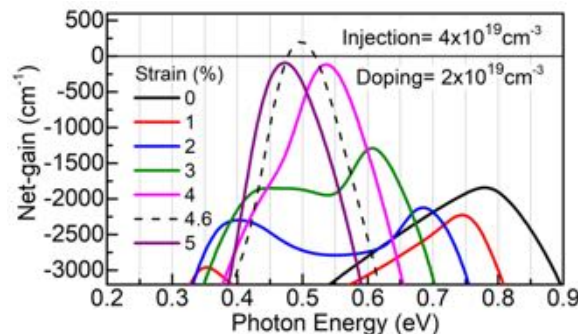


Fig. 10 Net-gain as a function of strain obtained after subtracting IVBA and eFCA from band to band gain.

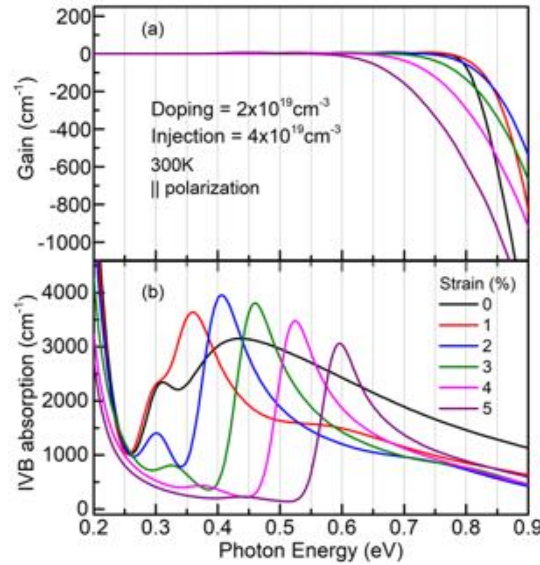


Fig. 11(a) Gain and (b) IVBA for light polarized parallel to strain. No band to band gain is available in this case.

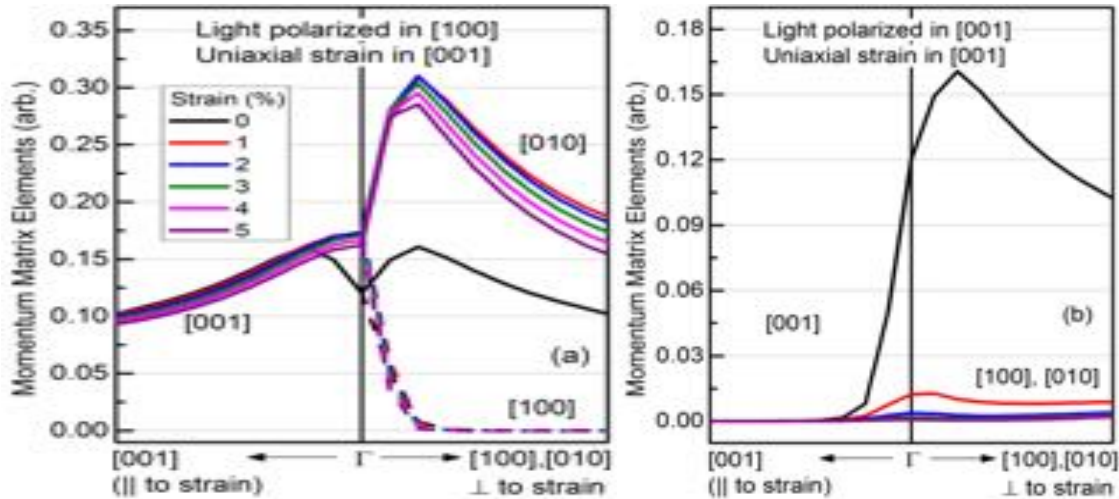


Fig. 12 Momentum matrix elements for VB1-CB1 transition; (a) Light polarized in [100] perpendicular to strain and (b) Light polarized in [001] parallel to strain

It should be noted that the net-gain until now was obtained by subtracting IVBA from gain. One other loss mechanism that needs to be considered is the free carrier absorption due to electrons (eFCA) in the conduction band. The basic difference between eFCA and IVBA is that eFCA increases smoothly with decreasing photon energy and does not have maxima and minima like features as was the case for IVBA [26]. This is because electrons cannot undergo vertical intra conduction-band transitions due to lack of available JDos close to emission photon energy [11]. It is well known that eFCA is based on a free electron effect i.e. the excited electron remains in the same energy band [26]. For free electrons to take part in intra-band absorption, conservation of

momentum and conservation of energy both need to be satisfied which is only possible through phonon scattering and ionized impurity scattering [26]. Since eFCA occurs in the same energy band through interaction of photons, phonons and dopant impurities, it is valid to assume that it will only depend on the shape of that band (i.e. effective mass), temperature, doping and carrier injection. Fig. 9 shows the effective mass of the Γ valley and L valley (both transverse and longitudinal mass) as a function of strain. It can be seen that the effective mass does not change appreciably in either valley as a function of strain. Therefore, for a given temperature, doping and carrier injection, eFCA can be expected to remain the same with strain. As such, an expression for eFCA fitted for bulk Ge [3] can be used for all strain values and the same has been used in this work. Fig. 10 shows the net-gain after subtracting both IVBA and eFCA from gain. It can be seen that, under the above operating conditions, positive net-gain is only available for uniaxial strain between 4% and 5% only when the special “resonance” between gain and IVBA takes place. Detailed modeling of IVBA uncovered this resonance for the first time and holds the key for a room temperature Ge laser. Our findings strongly suggest that hitting this resonance should be the goal of experimental work around s-Ge whereas the pursuit of direct band-gap Ge has been the main objective thus far.

1.4 EFFECT OF POLARIZATION AND ROLE OF MOMENTUM MATRIX ELEMENTS

In the last section, all the results were obtained for light polarized in a direction perpendicular to strain. Fig. 11 shows the gain and IVBA for light polarized parallel to strain direction. All the other simulation parameters are kept exactly the same as before. It is evident that there is no band-to-band gain available in this case which is remarkably different from the case when the light is polarized perpendicular to the strain as shown in Fig. 4. It proves that the polarization of light plays an important role in the process of light emission which is also shown experimentally in Ref. [5]. The shape of the IVBA curves is also significantly different between the two polarizations (compare Fig. 11(b) and Fig. 5). The effect of polarization is captured in the model by means of momentum matrix elements (MME) and since the effect is so large, it is imperative to study the matrix elements in detail. The matrix elements are calculated using the expression: $p_{12} = \langle \psi_1 | p | \psi_2 \rangle$ where ψ_1 and ψ_2 are the wave-functions of the bands 1 and 2 and p is the momentum operator. The diagonalization of the EPM Hamiltonian described in Section II yields not only the energy levels (eigenvalues) but also the eigenvectors which are nothing but the wave-functions in the reciprocal space with the basis set $\{G\}$. The wave-functions are then converted into real-space by means of a simple transformation. After calculating the wave functions, p_{12} is obtained by performing the above operation. This computation is done for transition from band 1 to 2 at all points in the FBZ and so we obtain $p_{12}(k)$.

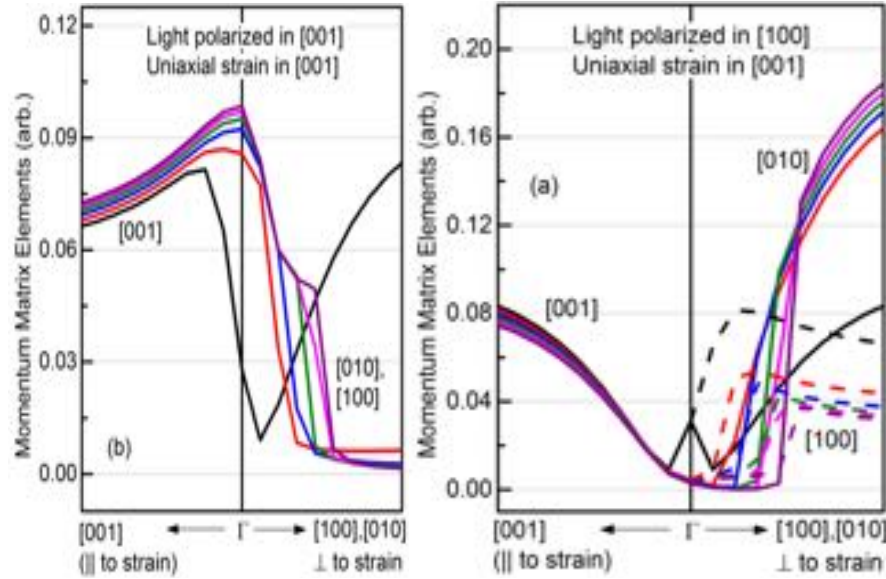


Fig. 13 Momentum matrix elements for SO-VB1 transition; (a) Light polarized in [100] perpendicular to strain and (b) Light polarized in [001] parallel to strain

Fig. 12 shows the momentum matrix elements for the VB1-CB1 transition computed as a function of reciprocal space vectors (k). The Γ point is taken as the origin and then the k -vectors are plotted in the direction parallel to strain axis ([001]) on left side and in directions perpendicular to strain ([100] and [010]) on the right side. For the transition, we consider light polarized perpendicular to strain (left graph) and light polarized parallel to strain (right graph). It can be seen that for light polarized in [100] direction perpendicular to strain (Fig. 12(a)), the momentum matrix elements are non-zero and large along [001] and [010] directions and tending towards zero only for [100] direction. When these matrix elements are introduced in the Fermi's Golden equation described before, it leads to a positive gain under certain conditions. On the contrary, for the light polarized in [001] direction parallel to strain (Fig. 12(b)), the matrix elements tend to zero for all three axes except for bulk Ge. This is the precise reason which explains absence of gain in s-Ge when light is polarized parallel to strain. It also proves that strain significantly changes the valence band character due to mixing effects and it is necessary to compute these matrix elements as a function of strain. Using the same values for s-Ge as computed for bulk Ge will lead to erroneous results. The difference between the shapes of IVBA curves for different polarization of light is explained by the MME for SO-VB1 transition. Fig. 13 shows the momentum matrix elements for SO-VB1 transition laid out in same way as Fig. 12. On close examination, it can be observed that the matrix elements for perpendicular and parallel polarization of light are complementary to each other. For [100] polarization the elements tend to zero when they are maximum for the case of [001] light polarization. Because of the complementary nature, the shape of the IVBA curve is highly dependent on the polarization of the light. Therefore, from Fig. 12 and 13 we can conclude that polarization of light plays a major role in underlying physics of light emission, more so, when valence band mixing effect takes place due to strain in the material.

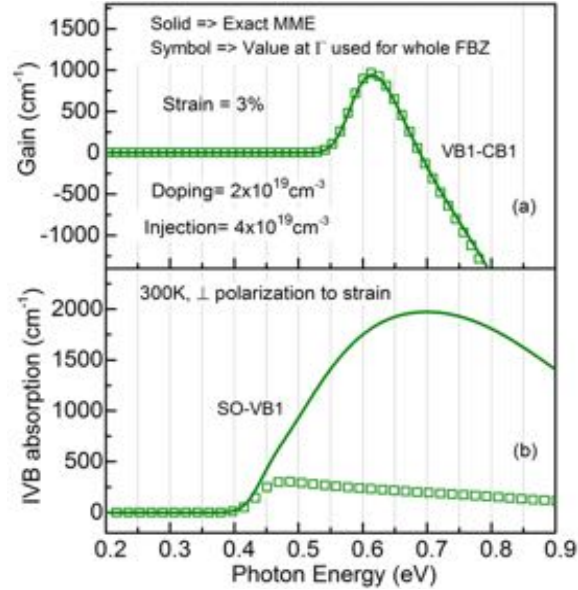


Fig. 14 Comparison of (a) gain and (b) IVBA for the case when momentum matrix elements at Γ is used for the complete FBZ and the case when the MME are evaluated separately at all points in FBZ which is the exact calculation.

Apart from the polarization of light, the dependence of matrix elements on k-vectors is also significant. The large variation in MME as a function of k-vectors can be established from Fig.13. In order to prove it further, Fig. 14 compares the gain and IVBA for the case when the value at Γ ($k=0$) is used for all points while integrating over the FBZ in Fermi's golden rule and for the case when the elements are evaluated separately for all k-points which is the exact computation. Fig. 14(a) compares the gain obtained for the two cases for the VB1-CB1 transition which is the major component of total gain. It is clear that the approximation of using MME at Γ for the complete FBZ is reasonable for gain calculation and it matches the exact computation well. This is because the MME's for VB1-CB1 transition does not vary significantly over the FBZ and also because only the k-points very close to Γ actually contribute to the gain. The same approximation is also used in Ref. [27] for gain calculations. On the contrary, IVBA is remarkably different between the two cases for the SO-VB1 transition. This is because the MMEs change by more than an order of magnitude between Γ and the k-points close to Γ as shown in Fig. 13(a). Moreover, with high injection levels required for achieving positive net-gain, the fermi level can be expected to go deep into the valence bands and hence a large number of SO-VB1 transitions can take place away from the Γ point. Thus it is imperative to account for the change in MME for the SO-VB1 transition as a function of k-points in order to capture the IVBA accurately.

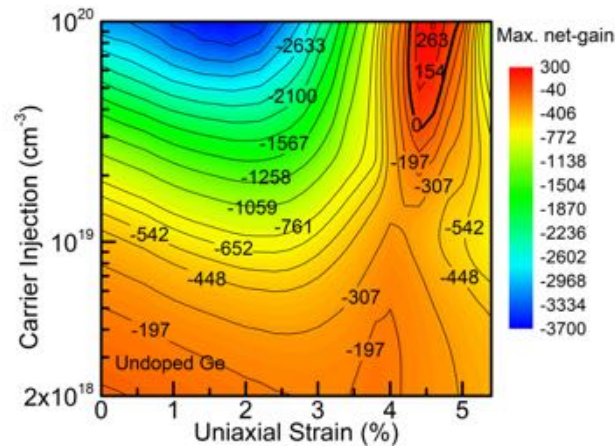


Fig. 15 Contour plot showing maximum net-gain as a function of strain and carrier injection. Ge is doped $1 \times 10^{19} \text{ cm}^{-3}$. Positive net-gain is achievable in a narrow window between 4-5% strain and injection above $2 \times 10^{19} \text{ cm}^{-3}$.

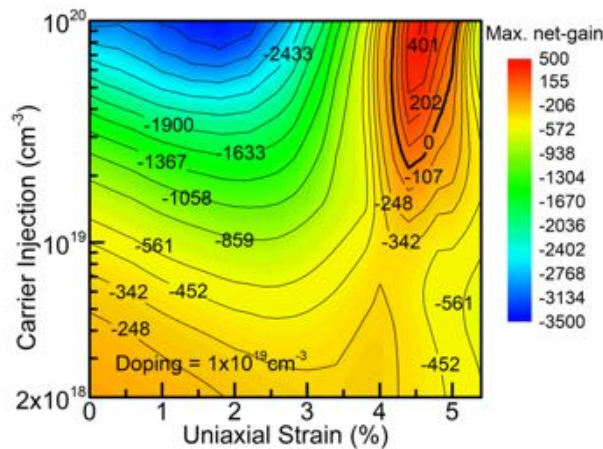


Fig. 16 Contour plot showing maximum net-gain as a function of strain and carrier injection. Ge is considered undoped. Positive net-gain is achievable in a narrow window between 4-5% strain and injection above $3 \times 10^{19} \text{ cm}^{-3}$.

1.5 EFFECT OF CARRIER INJECTION AND DOPING

In the last sections the role of strain and polarization of light was studied while keeping the carrier injection fixed at $4 \times 10^{19} \text{ cm}^{-3}$ and Ge doping at $2 \times 10^{19} \text{ cm}^{-3}$. In this section, the effect of carrier injection and doping in Ge is studied in conjunction with uniaxial strain while assuming the polarization of light to be perpendicular to strain. Fig. 15 is a color-map which shows the net-gain as a function of both strain and carrier injection with a fixed doping of $1 \times 10^{19} \text{ cm}^{-3}$. The desired area with a positive net-gain is demarcated with a bold black curve. It can be seen that positive net-gain is available only in a small window when the carrier injection is greater than $2 \times 10^{19} \text{ cm}^{-3}$ and the uniaxial strain is between 4-5% and. For carrier injection lower than $2 \times 10^{19} \text{ cm}^{-3}$ and/or strain less than 4%, the band-to-band gain is very small because of the indirect band-gap of Ge. In

addition, as discussed in Section III, at those strain levels the minima in IVBA does not align with the maximum in gain thereby incurring large absorption losses. For strain greater than 5%, gain and IVBA begin to come out of alignment (as shown in Section III) and that again leads to large losses. Therefore, it is evident that strain and carrier injection have a strong interplay and both of them together play a central role in determining the light emission characteristics of uniaxially s-Ge.

Fig. 16 is similar to Fig. 15 but Ge is considered to be undoped and therefore it brings out the significance of doping in Ge. The basic difference between doping and carrier injection is that doping adds only one type of carrier while carrier injection is bipolar. Therefore, n-type doping is useful in filling up the satellite L valley without adding holes in the valence band, thus reducing the IVBA losses for a given value of gain. However, adding more electrons than required also increases the eFCA and so there is an optimum in doping [28]. Adding unwanted electrons also lead to Auger recombination which can increase the lasing threshold significantly. Fig. 16 shows that the net-gain for a given strain and injection level is lower for undoped Ge as compared to n-doped Ge (Fig. 15). This is because the number of electrons in the conduction band for a given strain and carrier injection would be less for the case of undoped Ge as compared to n-doped Ge. For the case of undoped Ge a positive net-gain is still available between 4-5% strain but the window is narrower than for the case of doped Ge. A n-doping of $1 \times 10^{19} \text{cm}^{-3}$ in Ge is technologically possible by regular epitaxy and implantation methods and as shown in Fig. 15, the minimum carrier injection to achieve positive net-gain at that doping is $2 \times 10^{19} \text{cm}^{-3}$. Therefore, we can conclude that uniaxial strain in the range of 4-5%, carrier injection around $2 \times 10^{19} \text{cm}^{-3}$ and a doping of around $1 \times 10^{19} \text{cm}^{-3}$ are the best design parameters in order to achieve a room temperature Ge laser.

1.6 CONCLUSIONS

A rigorous model is used to prove that detailed analysis of IVBA is necessary to understand the loss mechanisms in s-Ge. Simple expression derived by fitting the experimental data for loss in bulk Ge is not sufficient and cannot be extrapolated to s-Ge. The model ascertains that a positive net-gain can be achieved only when the maxima in band-to-band gain aligns with the minima in the IVBA. This condition is predicted to occur for uniaxial strain between 4 and 5%, carrier injection greater than $2 \times 10^{19} \text{cm}^{-3}$ for Ge doped $1 \times 10^{19} \text{cm}^{-3}$ at room temperature. Notably, the requirement of direct band-gap material for positive net-gain is shown to be unnecessary. The impact of strain on the MME due to valence band mixing is shown to be important. It is also mandatory that MME is a function of reciprocal wave-vectors (k) while calculating IVBA. Apart from strain, carrier injection, doping and polarization play a key role in the carrier statistics of s-Ge. The model shows that the interaction between strain and parasitic absorption processes is critically important for the lasing process in tensile s-Ge. This substantially revises prior literature and builds a roadmap for a room temperature Ge light source.

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2. Experimental demonstration of a strained Ge light

19

source

2.1 Introduction

Photonic-integrated circuits (PICs) are a key enabler for the miniaturization of various technologies such as light detection and ranging (LIDAR) for autonomous vehicles [1], biochemical sensors [2] and chip-level optical communications [3]. However, the realization of fully functional PICs is currently limited by the absence of an efficient laser source on silicon (Si) [4, 5]. Approximately a decade ago, germanium (Ge) began attracting much attention as a potential gain medium for integrated group IV lasers [6]. Unlike Si, the energy difference between the direct Γ and indirect L conduction valleys of Ge is only 140 meV, and therefore it is possible to force some electrons to populate the direct Γ conduction valley and to create a population inversion in Ge [6]. By employing heavy n-type doping in $\sim 0.2\%$ biaxially strained Ge to assist with population inversion, optically and electrically pumped Ge-on-Si lasers have been demonstrated [7–9]. However, these lasers suffered from an extremely high lasing threshold current density ($\sim 280 \text{ kAcm}^{-2}$) that precludes practical integration. It was well known that intrinsic losses from free carriers were a major culprit for this inefficiency [6, 10], which other researchers identified more specifically as the inter-valence band absorption (IVBA) process from free holes [11, 12]. The IVBA was discussed in detail in the last chapter.

During the last few years, researchers have been making relentless efforts to overcome the drawback of indirect bandgap Ge through a variety of techniques. Among those, tin (Sn) alloying into Ge has shown great promise because GeSn alloy with a reasonably high Sn concentration ($>6.5\%$) can achieve a direct bandgap [13–18]. Recently, a Fabry-Perot type GeSn waveguide with 12.6% Sn demonstrated lasing with an optical pumping threshold density of 325 kWcm^{-2} at 20 K [16], and a couple of more successful demonstrations have since followed [17, 18]. However, the lasing threshold of those GeSn lasers was still too high to be practical, possibly owing to faster than desired non-radiative recombination processes [16]. On the other hand, the application of large mechanical tensile strain can also address the challenge of the indirect bandgap in Ge by fundamentally altering the bandstructure [19–25]; the small energy difference between the Γ and L conduction valleys can be reduced even further with tensile strain, resulting in an increased material gain [24, 25]. This hypothesis has been supported by numerous theoretical simulations that predict a significant reduction in lasing threshold through tensile strain [10, 26]. With regard to practical realization, several innovative platforms for inducing large mechanical strain have been experimentally demonstrated [19–23], thus suggesting the possibility of low-threshold group IV lasers.

While lasing from highly strained Ge has been pursued intensively in several recent reports [27–33], there has been no successful demonstration of optical amplification in such a seemingly promising material system. Most notably, El Kurdi et al. [29, 31] investigated photoluminescence from direct bandgap Ge under a 1.75% biaxial tensile strain; however, no lasing action was observed even at cryogenic temperatures, possibly owing to a non-uniform strain distribution in the gain medium and/or a poor thermal conduction arising from suspended structures. The authors also performed theoretical calculations on the actual device temperature under the same pump conditions used in their measurements [23], and found that the temperature rises to 210 K which is significant enough to preclude lasing because of

the increased material loss. This temperature-dependent optical characteristic is discussed theoretically and experimentally throughout this study.

Here, the observation of low-threshold lasing from Ge nanowires under 1.6% uni-axial tensile strain is presented. With a pulsed optical pumping threshold density of $\sim 3.0 \text{ kWcm}^{-2}$ that is two orders of magnitude lower than the state-of-the-art Ge-based lasers [8, 16], we observe an unambiguous multimode lasing action evidenced by clear threshold behaviors in output power and linewidth as a function of pump power. Theoretical modeling shows that the IVBA, the recently discovered dominant loss factor in Ge [11, 12, 33], is markedly reduced at cryogenic temperatures [34] and therefore can be compensated by the amplified material gain in strained Ge, leading to the development of a large optical net gain of $\sim 415 \text{ cm}^{-1}$. By presenting unambiguous quantitative evidence of low-threshold lasing action in a fully CMOS-compatible material system, our results pave the way towards a monolithic realization of PICs.

2.2 Germanium-on-insulator (GOI) substrate preparation

The strained Ge nanowire laser demonstrated in this work makes use of a GOI substrate. The fabrication process flow for this GOI stack is depicted in Fig.4.1. The advantages of such a stack will become evident in subsequent sections. First, a $2.2 \text{ }\mu\text{m}$ thick Ge layer with an n-type dopant concentration of $1 \times 10^{19} \text{ cm}^{-3}$ was grown on a Si substrate using multiple hydrogen annealing heteroepitaxy (MHAH) [35]. A 25 nm thick Al_2O_3 sacrificial layer was then deposited using atomic layer deposition (ALD). A Si carrier wafer with an 850 nm thick SiO_2 layer was prepared by thermal oxidation at 1100°C . After wet-chemical treatment of the two bonding surfaces (Al_2O_3 and SiO_2), the two wafers were directly bonded at room temperature, followed by a high-temperature anneal to increase bonding strength. The Si substrate of the carrier wafer was then selectively etched away using TMAH, stopping at the Ge layer. By using chemical-mechanical polishing (CMP), the Ge layer was thinned down to 200 nm , finalizing the fabrication process for the substrate. Although this fabrication process involves wafer bonding, the bonding step does not require any alignment and is comparable in complexity to current industrial-scale silicon-on-insulator (SOI) processes.

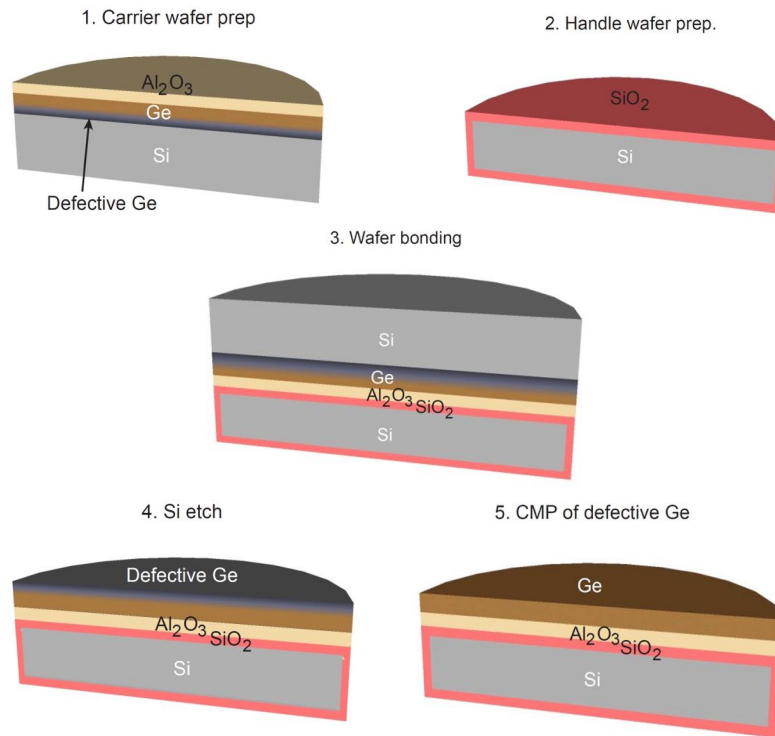


Figure 4.1: Schematics of the germanium-on-insulator (GOI) substrate fabrication process.

2.3 Fabrication of uniaxially strained devices on Ge

In this section, two different methods to introduce high uniaxial strain in Ge are discussed. The first method utilizes the high intrinsic tensile strain engineered in as-deposited Silicon Nitride (SiN) films. The second method relies on the amplification of the small $\sim 0.2\%$ biaxial strain in Ge grown on Si.

Strained Ge through SiN stressors

Fig.4.2(a) shows a schematic of the proposed structure for the first method. The main component is a suspended Ge beam which needs to be subjected to tensile strain to make it an efficient gain material. This is achieved by attaching two transverse SiN beams with inherent tensile strain and then allowing them to relax while keeping their ends fixed as shown in Fig.4.2(a). As the SiN beams relax, they pull on the Ge beam so as to induce a large tensile strain in the active region between the stressors. More details on the physical realization of this structure will be discussed in the next paragraph. The optical cavity can be designed around the s-Ge active medium and consists of circular photonic crystal holes in the schematic. Such suspended beams have already been studied in other material systems for high quality factor optical

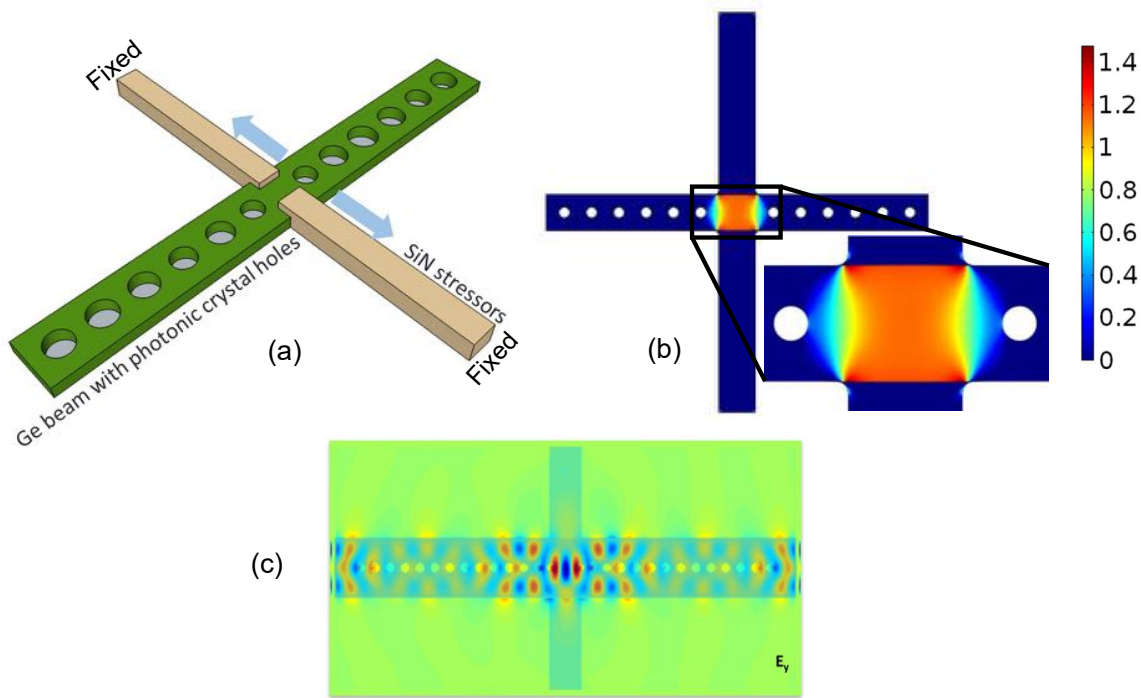


Figure 4.2: (a) Schematic of the proposed structure showing different components,

Finite element method (FEM) modeling of the strain profile in the structure and Finite difference time domain (FDTD) simulation of the proposed optical cavity showing a quality factor greater than 11,000 and a small mode volume of $1.8(\lambda/n)^3$

cavities with small mode volumes [36] and can be readily applied to our own structure. Fig.4.2(b) shows the simulated strain profile calculated using finite element method (FEM) COMSOL modeling of the structure described above. High tensile-strain concentration (as high as 1.25% from simulations) is evident at the center of the Ge beam. The zoomed-in portion of Fig.4.2(b) shows that the circular photonic crystal holes have no adverse effect on the strain profile and the strained SiN beams and the proposed optical cavity can readily co-exist.

The actual design of the optical cavity involved calculating the optimal size and spacing of the circular holes for the intended wavelength. Finite difference time domain (FDTD) simulations, shown in Fig.4.2(c), were carried out on the proposed structure and a strong optical confinement within the s-Ge gain medium can be clearly seen. The quality factor and mode volume of the optical cavity for this ideal structure (no surface roughness and lossless gain medium) were evaluated to be $>11,000$ and $1.8(\lambda/n)^3$, respectively. Thus, the proposed structure has an s-Ge gain medium bounded by high reflectivity mirrors on both sides to constitute a high quality optical cavity, thereby satisfying the basic requirements of a low threshold Ge laser.

The process flow for s-Ge beams is shown in Fig.4.3. To begin, a Ge beam is patterned by e-beam lithography (EBL) and anisotropic dry etching on a germanium-on-insulator (GOI) substrate. The material stack for the initial GOI substrate consists of Si/SiO₂/Al₂O₃/Ge, as discussed in the last section. A SiN film is deposited through LPCVD and patterned using EBL, which then constitutes the transverse SiN beams, as shown in Fig.4.3. The stress in the

LPCVD SiN films can be engineered to achieve large-tensile strains with the appropriate deposition conditions [37]. However, since these patterned SiN beams are still attached to the exposed Al_2O_3 of the GOI material stack, they are not free to move and need to be released before they can transfer any substantial strain to the Ge beam. This release is accomplished by selectively under-etching the Al_2O_3 using KOH which does not etch SiN or the Ge beam. In this way the SiN stressors become suspended which allows them to relax, transferring strain to the Ge beam as a result. The SEM image of the fabricated device is shown in Fig.4.4(a). We also consider an alternate design with larger strain elements, shown in Fig.4.4(b), which is expected to transfer more strain to the Ge beam based on

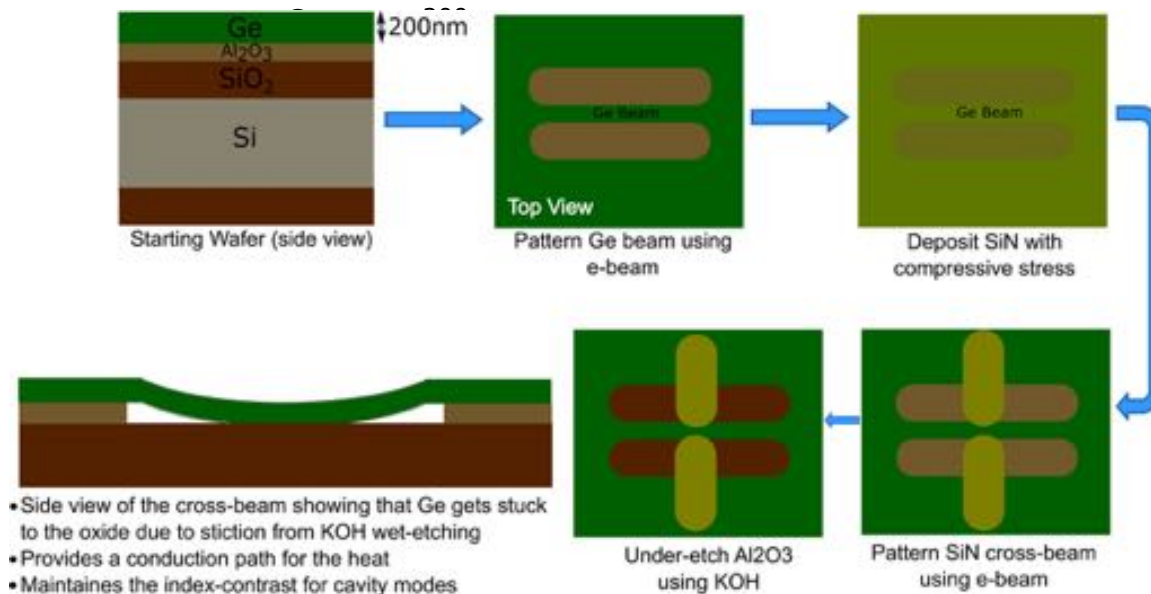


Figure 4.3: Schematic showing the process flow for the fabrication of strained Ge beams using silicon nitride.

our FEM studies. The actual tensile strain distribution in both Ge beam designs was then experimentally measured using Raman spectroscopy as described in [20]. Raman line scans for the two device structures are shown in Fig.4.4(c). The Raman spectrum is measured at the center of the strained region in the beams. The absolute amount of strain achieved in the active region with the structures of Fig.4.4(a) and Fig.4.4(b) was measured to be 1.27% and 1.70%, respectively. A 2D area scan of the peak Raman shifts, shown in Fig.4.4(d), confirms that the beam is highly strained in the active region between the SiN stressors. This strain is also highly localized, with a small but non-zero Raman shift observed elsewhere in the Ge beam because of the initial strain in the GOI substrate [20]. The strain can be further increased controllably by increasing the SiN stressor length and width, allowing excellent design flexibility and customizability at the lithography level.

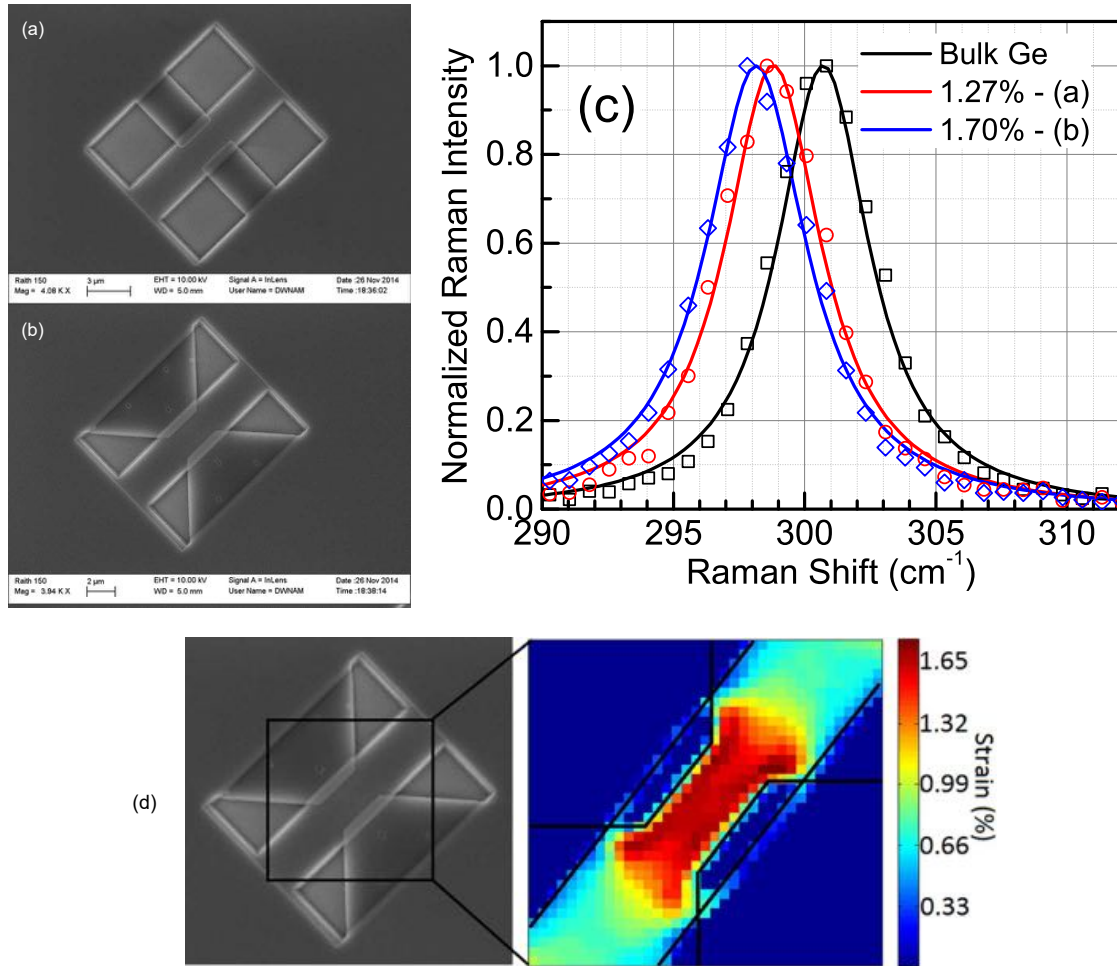


Figure 4.4: (a) SEM of the structure showing Ge beam and SiN stressor, (b) A different design which maximizes the SiN stressor volume in order to transfer more strain in the Ge beam, (c) Raman spectra measured at the center of Ge beam for structures in (a) and (b), (d) 2D mapping of the peak Raman shifts measured in structure (b) showing a large strain in the active region of the Ge beam.

Strained Ge through amplification of inherent tensile strain

In this section, another method of introducing large uniaxial tensile strain in Ge using strain amplification technique is demonstrated. The process flow is shown using schematics in Fig.4.5. The device is fabricated in a material stack consisting

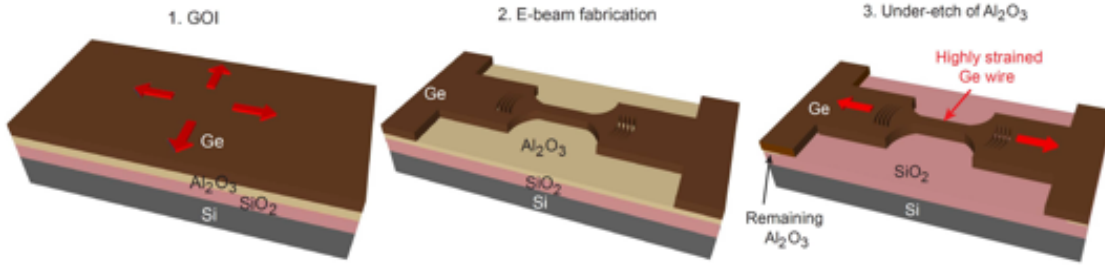


Figure 4.5: Schematic showing the process flow for the fabrication of strained Ge beams using amplification of intrinsic biaxial strain in Ge on Si films.

of four layers: 200 nm Ge, 25 nm Al_2O_3 , 850 nm SiO_2 , and Si wafer, as discussed in the last section. The Ge layer is n-type doped with $1 \times 10^{19} \text{ cm}^{-3}$ phosphorus atoms using in situ doping during growth. The device is patterned using a single electron beam lithography step, followed by a HBr/Cl_2 dry etch for pattern transfer to the Ge layer. The structure is then undercut by a KOH wet etch to selectively remove the Al_2O_3 layer, releasing the very slightly (0.2%) strained Ge layer from the substrate. This step allows the large pads to contract, amplifying the strain in the nanowire [20, 21, 23]. The curved trenches etched on either side of the Ge nanowire represent high quality factor DBR mirrors designed to act as a cavity for the laser structure. Specific details of these DBR mirrors will be discussed subsequently.

Fig.4.6 presents a scanning electron micrograph (SEM) of a fabricated device, consisting of an $8 \mu\text{m}$ long highly strained Ge nanowire surrounded by two large pads containing distributed Bragg reflector (DBR) mirrors which form the optical cavity. While crucial for inducing strain in the nanowire, the undercut creates an air gap between the Ge layer and the substrate, severely limiting thermal conduction out from the nanowire and resulting in the destruction of devices under optical pump powers of $\sim 5 \text{ mW}$. To address this limitation, we make use of capillary forces to pull the Ge nanowire down and bring it into contact with the SiO_2 layer when drying the device after the undercut step. The nanowire is then held in contact with the SiO_2 layer by van der Waals forces. The SiO_2 layer enables optical confinement in the Ge while also serving as an additional heat conduction path, permitting a $> 10\times$ increase in pump power.

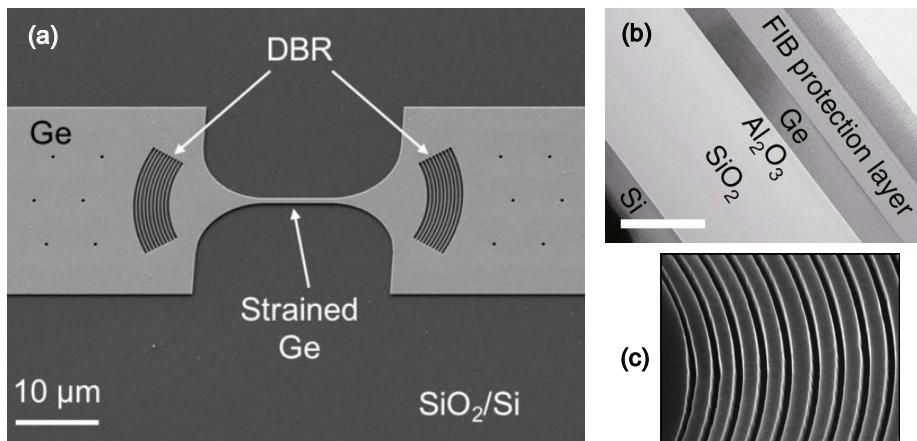


Figure 4.6: Strained Ge nanowire. (a) Scanning electron micrograph (SEM) of a fabricated device, showing the etched Ge nanowire and adjacent distributed Bragg- reflector (DBR) mirrors, (b) Side-

view SEM of the initial Ge-on-insulator material stack. Scale bar - 500 nm and (c) Detailed view of the DBR mirrors.

The measured 2D Raman map of the device is shown in Fig.4.7(a). It is evident that the strain is uniformly distributed across the length of the nanowire. Additionally, because tensile strain reduces the bandgap of Ge, the spatial variation in the strain profile creates a pseudo-heterostructure which confines carriers to the nanowire region, greatly improving carrier concentrations in the gain medium [21]. Moreover, the amount of strain can be changed by changing the length ratio of the wire and the pads. The longer the pads with respect to the wire, the larger will be the strain in the nanowire. This property is demonstrated in Fig.4.7(b), where Raman line-scans are shown for devices with different length ratios between the wire and the pads. Clearly, the strain in the nanowire can be tuned to a desired value in a broad range.

Using finite difference time domain (FDTD) optical simulations (Fig.4.8), a device that supports optical modes with radiative quality factors of over 10^4 while retaining very high mechanical strain along the nanowire was designed. The straight 8 μm long 700 nm wide active region is expanded to a maximum width of 13.7 μm and then connected to 20 μm wide side pads. The total distance between mirrors is $\sim 30 \mu\text{m}$. 10-period DBR mirrors with a period of 380 nm and a nominal duty cycle of 21% are matched to the shape of the optical mode. Due to the small dimensions of the nanowire, the structure supports no higher-order transverse modes.

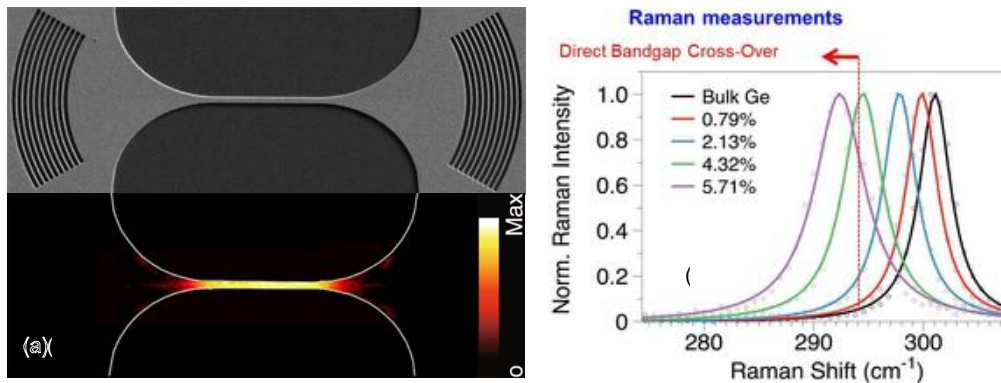


Figure 4.7: (a) Strain map for a fabricated device, experimentally obtained using Raman spectroscopy and (b) Raman line-scans at the center of strained devices with different length ratios between the wire and the pads.

Fig.4.9(a) shows photoluminescence spectra from unstrained, 1.95%, and 2.37% strained nanowires with identical optical cavities. The devices were pumped with

2.5 mW of power from a continuous-wave (CW) 980 nm diode laser. The emission peak can be seen to redshift from ~ 1560 nm to at least 1980 nm as the strain in the nanowire increases and the bandgap narrows [38]. The position of the emission peak for the 2.37% strained nanowire artificially appears at a shorter wavelength than

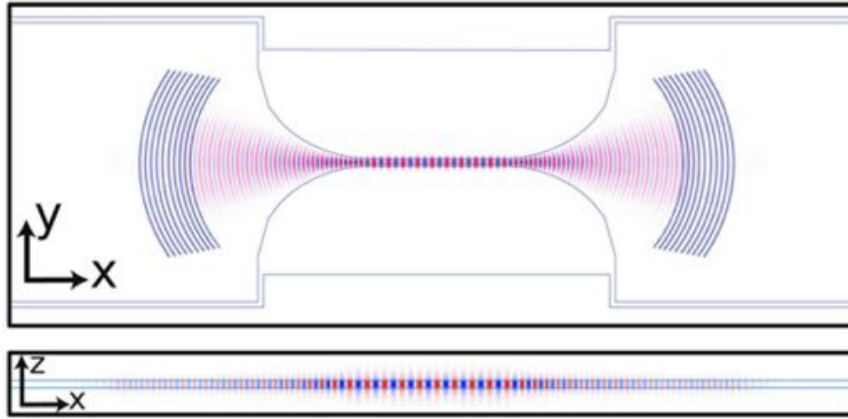


Figure 4.8: Ey field distribution for the optical mode with a free-space wavelength of 2 μm , obtained with FDTD simulation.

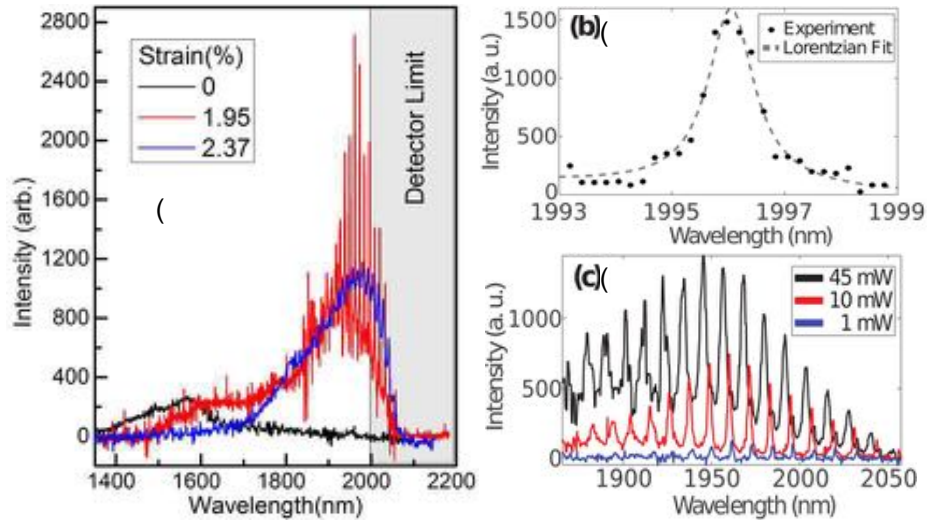


Figure 4.9: (a) Photoluminescence (PL) spectra for devices with 0%, 1.95%, and 2.37% tensile strain. The detection limit of the spectrometer is denoted with a gray background. (b) Lorentzian fit to a single resonance peak with fitted quality factor of 2020. (c) High resolution PL spectra for a 1.95% strained nanowire pumped with increasing average power from a pulsed laser source.

expected (>2000 nm) due to a gradual reduction in signal intensity caused by the detection limit of the extended InGaAs photodiode array used to collect the spectra. Optical resonances with a free spectral range of 24.6 nm are visible in the strained wire spectra but are obscured by noise in the unstrained wire spectrum due to low signal intensity. Fig.4.9(b) presents a Lorentzian fit to a single optical mode under identical pump conditions. A Q-factor of 2020 is observed, limited by sidewall roughness along the nanowire and material absorption. Fig.4.9(c) shows the spectra from a 1.95% strained nanowire under pulsed excitation with various average powers. The pulsed pumping source was a 1550 nm laser with 2 μs pulse period and 200 ns pulse length, chosen to minimize heating.

Contrary to previous reports [7, 8], signs of lasing, such as line width narrowing were not observed,

although our material is highly strained and has a similar doping level to the reported optically pumped Ge-on-Si laser. The net optical gain for 2.37% ($\lambda = 2010$ nm) and 1.95% ($\lambda = 1923$ nm) strained nanowires is shown in Fig.4.10(a). The net gain decreases with increasing pump power, indicating that increasing free-carrier losses overwhelm any optical gain from the direct-band transition. Nevertheless, we find a significant improvement in net gain as the strain is increased from 1.95% to 2.37%, likely due to an increase in the available optical gain. To model the net gain present in our structures, we first use the empirical pseudo-potential method (EPM) to evaluate the band structure of strained Ge. EPM is known to capture the effects of strain on band structure, including the valence band splitting, particularly well [39]. Exactly the same model as discussed in the last chapter is used to model the gain and IVBA for the present experimental setup. By fitting this model (Fig.4.10(b), dashed line) to our calculated experimental net gain, we extract a minority carrier lifetime of 2.9 ns, in good agreement with previous measurements [40].

By increasing strain from 1.95% to 2.37%, we observed a significant reduction in net optical loss, in agreement with the predictions of our model. Extension of our model to higher strain values suggests that net positive gain can be achieved in $\sim 4\%$ strained Ge at room temperature for a doping of $1 \times 10^{19} \text{ cm}^{-3}$ and carrier injection of approximately $2 \times 10^{19} \text{ cm}^{-3}$. This is a consequence of complex valence band splitting in the very high strain regime, as shown in great detail in the last chapter. As strain values in excess of 5% have been observed experimentally [23], we expect that extension of this work to devices capable of sustaining 4% or higher tensile strain will enable low-threshold room temperature lasing in Ge.

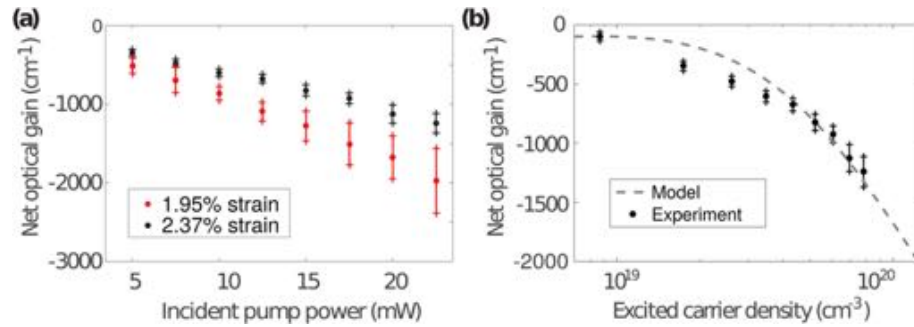


Figure 4.10: (a) Plot of net optical gain versus incident pump power (980 nm CW) for 2.37% (black, $\lambda = 2010$ nm) and 1.95% (red, $\lambda = 1961$ nm) strained nanowires, (b) Net optical gain versus injected carrier density for the 2.37% strained device. Black dots indicate experimental data, and the dashed gray line indicates values from EPM calculations.

2.4 Low temperature laser demonstration

The structure described in the section above was then extensively studied at low temperatures. The DBR mirrors were further optimized to minimize optical loss. Multimode lasing by optically exciting a 1.6%-strained Ge nanowire integrated with DBRs at a temperature of 83 K was observed. Fig.4.11(a) presents the emission spectra from the laser structure at different pump powers. A linear polarizer inclined perpendicular to the nanowire axis is placed in front of the spectrometer to investigate polarization-dependent lasing behaviour. At a low pump power of 0.7 kWcm^{-2} , the emission shows broad spontaneous emission which consists of two overlapping peaks arising from optical transitions of Γ -VB1 and Γ -VB2 [28, 38]. At an increased pump power of 1.4 kWcm^{-2} , visible longitudinal cavity modes owing to the presence of DBRs emerge on the long wavelength side as the

optical loss is gradually compensated by the material gain. Although such cavity modes near the band edge from highly strained Ge have been already observed numerous times [28–33], all the previous reports showed the apparent intensity saturation and linewidth broadening of cavity modes with pump powers possibly owing to insufficient gain at low strain [30, 32], poor optical cavity [28, 29] and/or unsatisfactory thermal management [29, 33].

In the present study, on the other hand, the cavity modes near the band edge attain a superlinear increase in intensity along with a significant linewidth reduction as the pump power is increased to 3.5 kWcm^{-2} . This phenomenon clearly presents the evidence of optical amplification in highly strained Ge gain medium. Interestingly, the spontaneous emission well above the band edge ($<1550 \text{ nm}$) also collapses into sharp cavity modes, thus suggesting that the entire emission band is close to the transparency condition. The full-width at half-maximum (FWHM) of the emission band at this pump power is $\sim 150 \text{ nm}$. The mode spacing is measured to be $\sim 8 \text{ nm}$, which is consistent with FDTD simulations. Optical simulations also confirm that a fundamental transverse mode can be confined within a Ge nanowire with cross-sectional dimensions of $700 \text{ nm} \times 220 \text{ nm}$ (width $\times$ height). It is worth mentioning that the occurrence of amplified cavity modes over the whole emission band is in stark contrast to conventional lasing materials for which cavity modes are generally observed only within a relatively narrow gain bandwidth. This unique behavior in highly strained Ge will be explained in the following gain modeling section.

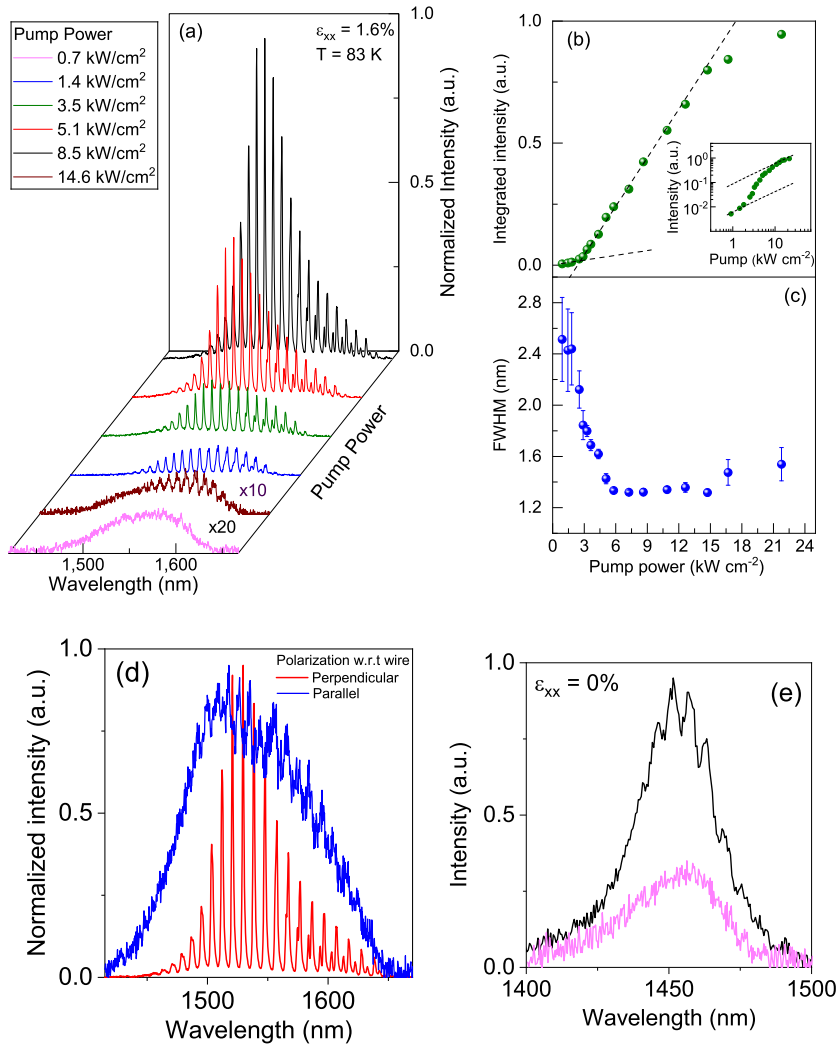


Figure 4.11: (a) Power-dependent photoluminescence spectra of a 1.6%-strained Ge nanowire with distributed Bragg reflectors (DBRs) showing a gradual transition from broad spontaneous emission to multimode lasing oscillation, (b) Integrated photoluminescence intensity vs. optical pump power. Inset: corresponding double-logarithmic plot showing nonlinear response to pump power represented by an S-shaped curve, (c) The linewidth evolution of the lasing mode at 1530 nm as a function of pump power, (d) Normalized polarization-dependent spectra collected at 14.6 kWcm^{-2} , showing a highly anisotropic gain property of strained Ge nanowires, (e) Photoluminescence spectra of the unstrained structure taken at 0.7 kWcm^{-2} (magenta) and 14.6 kWcm^{-2} (black) pump powers, showing no lasing action. The spectrum for the pump power of 0.7 kWcm^{-2} is multiplied by a factor of 3.

At higher pump powers of 5.1, 8.5, and 14.6 kWcm^{-2} , only the modes near 1530 nm continue growing rapidly in intensity as they enter the lasing regime while the modes near the band edge ($>1600 \text{ nm}$) appear to saturate. At the highest pump power of 14.6 kWcm^{-2} , the cavity modes near 1530 nm obtain $>20 \times$ higher intensity than the background spontaneous emission, and exhibit a well-defined bell-shaped curve following the net gain spectrum with the FWHM bandwidth of $< 50 \text{ nm}$ while the bandwidth of the background emission is $\sim 150 \text{ nm}$. The large bandwidths of both spontaneous emission [28, 29, 38] and net gain have been previously observed in highly strained Ge, and can be attributed to the unusually large amount of strain-induced valence band splitting ($\sim 72 \text{ meV}$ for 1.6%

uniaxial strain). The FWHM of a single- cavity mode at 1530 nm is determined to be ~ 1.3 nm by fitting to an individual Lorentzian function, corresponding to a Q-factor of >1100 .

Lasing action can also be quantitatively evidenced by the nonlinear behavior of the integrated output intensity within the gain bandwidth as a function of pump power (Fig.4.11(b)). The output intensity shows a superlinear growth near the threshold pump power (3.0 kWcm^{-2}) followed by a linear growth in the lasing regime, which clearly indicates a distinctive lasing action. The corresponding double-logarithmic plot of the output intensity dependence on the pump power (Fig.4.11(b), inset) manifests a typical nonlinear threshold behavior. By employing the multimode laser rate equation to fit our experimental data, we obtain a spontaneous emission factor, β , of ~ 0.08 . Fig.4.11(c) illustrates the linewidth evolution of the highest lasing mode at 1530 nm as a function of pump power. The linewidth reduces from ~ 2.5 nm to ~ 1.3 nm above the threshold pump power. The linewidth and the corresponding Q-factor at the threshold pump power of $\sim 3.0 \text{ kWcm}^{-2}$ is ~ 1.8 nm and $Q \sim 850$, respectively, assuming the effective index of 3.2 which is calculated from FDTD simulations. This simulated effective index is also consistent with the reported value in a recent work presenting strained Ge laser structure [29]. The threshold gain is estimated to be 336 cm^{-1} with the simulated optical confinement factor of 0.45. Above 15 kWcm^{-2} , the output intensity starts saturating while the linewidth broadens, which can be attributed to the sample heating. This challenge may be overcome by enhancing the thermal conductivity of the Ge nanowire structure by replacing the underlying insulating layer with a more thermally conductive material such as silicon nitride (SiN) and aluminium oxide (Al_2O_3).

The polarization dependence of the laser emission is also investigated as shown in Fig.4.11(d). The emission polarized parallel to the nanowire axis (blue) does not show evidence of optical amplification, manifesting a strong anisotropic gain property caused by uniaxial tensile strain.

Fig.4.11(e) presents the emission spectra from an unstrained Ge nanowire for 0.7 kWcm^{-2} (magenta) and 14.6 kWcm^{-2} (black). The emission spectrum at 0.7 kWcm^{-2} is broad and does not exhibit clear cavity resonances, similarly to the spectrum from the 1.6%-strained Ge nanowire under low pumping (magenta curve of Fig.4.11(a)). While the cavity resonances from the 1.6%-strained nanowire grow rapidly and dominate the background emission at higher pump powers due to the presence of optical net gain (black curve of Fig.4.11(a)), the unstrained nanowire shows only a slight modulation of the emission spectrum at 14.6 kWcm^{-2} , resulting in the dominant background emission over the cavity resonances. Theoretical modeling is performed for a comprehensive understanding of the gain and loss dynamics in the strained Ge material system. We use the empirical pseudopotential method (EPM) for computing the band structure of highly strained Ge, and numerical analysis is employed to calculate the material gain via Fermi's golden rule, as discussed in detail in the last chapter. For IVBA, we use experimentally extracted absorption cross-sections for room temperature [11, 20] and cryogenic temperature [34]. The loss is the sum of free electron absorption (FEA) and IVBA, and IVBA is the dominant factor as previously discovered in Refs. [11, 12]. At $7 \times 10^{19} \text{ cm}^{-3}$ carrier density, IVBA is 214 cm^{-1} whereas FEA is $\sim 96 \text{ cm}^{-1}$ for the experimental gain peak wavelength of ~ 1530 nm, thus making IVBA the major loss mechanism.

Fig.4.12(a) shows the calculated material gain with reverse sign (solid lines) and loss (dashed lines) at 83 K for three different carrier injection densities of $4 \times 10^{19} \text{ cm}^{-3}$ (blue), $5 \times 10^{19} \text{ cm}^{-3}$ (green) and $8 \times 10^{19} \text{ cm}^{-3}$ (red). At an injection density of $4 \times 10^{19} \text{ cm}^{-3}$, the material gain attains its peak intensity above 1600 nm, which corresponds to the optical transition between the Γ conduction valley and the top valence band, VB1. As the injection density is increased to $5 \times 10^{19} \text{ cm}^{-3}$, a large number of holes start filling up the second valence band, VB2, resulting in the emergence of another gain peak below 1600 nm. The significantly increased gain bandwidth extends down to

~1500 nm, thus explaining the experimental observation of cavity modes within such a large spectral range for the spectrum taken at 3.5 kWcm^{-2} in Fig.4.11(a). The gain continues increasing at an injection density of $8 \times 10^{19} \text{ cm}^{-3}$ and allows the achievement of a large optical net gain of $\sim 415 \text{ cm}^{-1}$ at $\sim 1510 \text{ nm}$. The gain for unstrained Ge at an injection density of $8 \times 10^{19} \text{ cm}^{-3}$ (black solid line) is overwhelmed by the loss for the same injection density (red dashed line), highlighting the significance of tensile strain for obtaining optical net gain in Ge.

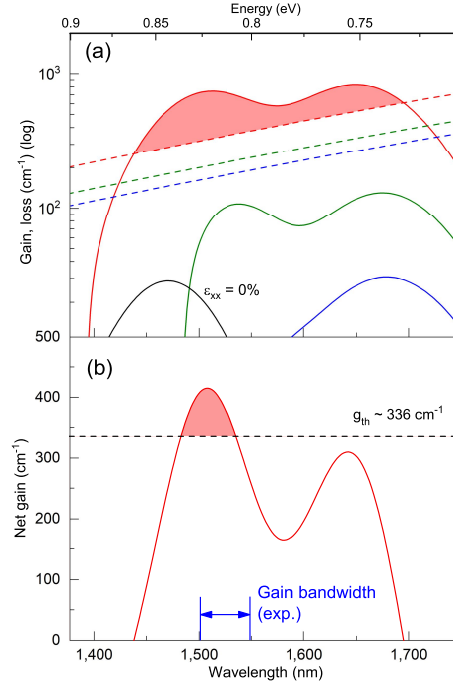


Figure 4.12: (a) Calculated gain (solid line) and loss (dashed line) for 1.6% strained Ge at injection densities of $4 \times 10^{19} \text{ cm}^{-3}$ (blue), $5 \times 10^{19} \text{ cm}^{-3}$ (green) and $8 \times 10^{19} \text{ cm}^{-3}$ (red). The gain for unstrained Ge at an injection density of $8 \times 10^{19} \text{ cm}^{-3}$ (black solid line) is overwhelmed by the loss, (b) Calculated net gain spectrum for an injection density of $8 \times 10^{19} \text{ cm}^{-3}$.

Fig.4.12(b) shows the net gain spectrum obtained by subtracting the loss from the gain for an injection density of $8 \times 10^{19} \text{ cm}^{-3}$. Although there exist two gain bands associated with optical transitions of Γ -VB1 and Γ -VB2, the gain band centered at $\sim 1510 \text{ nm}$ only surpasses the experimental threshold gain of 336 cm^{-1} . The measured gain bandwidth is also presented as a blue arrow, which is in reasonable agreement with the theoretical gain bandwidth. The slight discrepancy between the theoretical and experimental gain bandwidths may be ascribed to the uncertainty in band structure calculation for such highly strained Ge.

Fig.4.13 presents the integrated output intensity of the 1.6%-strained Ge nanowire as a function of the pump power at different temperatures of 83, 123 and 173 K. While at 83 K, optical amplification enables the output intensity to grow superlinearly near the threshold, the data sets for 123 and 173 K do not show such a clear nonlinear threshold behavior. It should be noted that a clear saturation of the output intensity for 123 and 173 K was observed at higher pump powers owing to the absence of optical net gain. The inset shows the normalized emission spectra taken at 83 K (green) and 173 K (black) at a pump power of 14.6 kWcm^{-2} . In contrast to the spectrum for 83 K showing the dominant lasing modes over the background spontaneous emission, the cavity modes are highly suppressed at

173 K and do not show a superlinear growth in intensity at higher pump powers, which displays a strong temperature dependence of gain characteristics in strained Ge. The gain and loss analysis for 300 K shows that optical net gain is not achievable in 1.6%-strained Ge owing to a substantial IVBA, thus highlighting the significant role of IVBA in realizing Ge lasers.

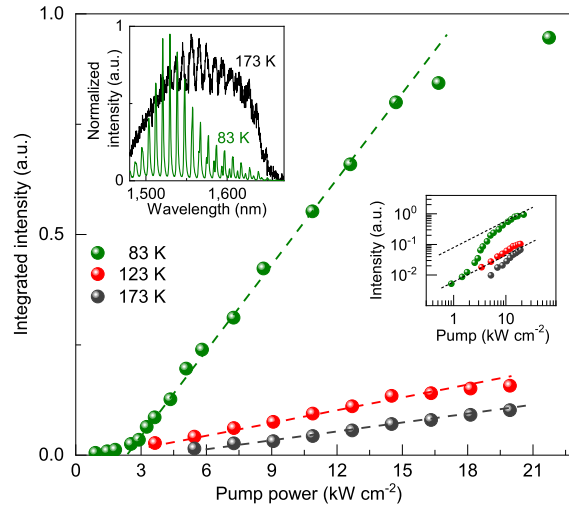


Figure 4.13: Integrated output intensity vs. pump power of a 1.6% strained structure at temperatures of 83 K (green), 123 K (red) and 173 K (black). Right inset: corresponding double-logarithmic plot for 3 temperatures. Left inset: normalized emission spectra collected at 83 K (red) and 173 K (black) under a pump power of 14.6 kW cm^{-2} .

Theoretical studies presented in the last chapter predicted that room-temperature lasing can be achieved from $>4\%$ strained Ge because of the further amplified material gain. Since higher than 4% uniaxial tensile strain has been already achieved in Ge nanostructures, we anticipate that the further development of our laser structure will certainly enable us to obtain such highly strained Ge gain media coupled with high-Q optical cavity for the realization of room-temperature Ge lasers.

2.5 Conclusion

In summary, we have demonstrated lasing from highly strained Ge nanowires. Our nanowire laser design secures robust mechanical, optical, and thermal properties, which played major roles in enabling low-threshold lasing from highly strained Ge. Excitation, temperature, and polarization dependent optical characterizations showed the achievement of pulsed lasing at 83 K with an optical pumping threshold density of 3.0 kW cm^{-2} , the lowest value among group IV lasers reported to date [7–9], [16–18]. Room temperature lasing could be achieved in our architecture, but with a higher level of tensile strain that is within reach [12, 20, 23]. We believe that single mode operation can be realized by further optimizing the cavity through the use of shorter optical cavities or employing distributed feedback (DFB) gratings. The realization of a low threshold, electrically pumped Ge laser is also possible by using a lateral p-i-n junction [41]. In addition, the ability to tune the strain conveniently by a conventional lithography [20, 21, 42] should enable the creation of multiple lasers operating at different spectral ranges on a single chip, which is crucial for wavelength division multiplexed optical interconnects. Our demonstration of a low-threshold, highly strained Ge

nanowire laser markedly narrows the gap between conventional III-V lasers and their group IV counterparts, thus opening up new avenues for PICs.

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3. Silicon-Compatible Fabrication of Inverse Woodpile Photonic Crystals with a Complete Band Gap

3.1 INTRODUCTION

Complete control of photons in all three dimensions is considered to be the holy-grail of photonics. It is well understood that such a complete control is possible only through three-dimensional (3D) photonic crystals with a complete band gap [1-14]. For a given range of frequencies, such photonic crystals forbid the propagation of electromagnetic radiation for all wave-vectors and hence can have a profound impact on the optical behavior of materials. Of the multitude of applications of 3D photonic crystals, the most interesting are - (a) complete inhibition of spontaneous emission for frequencies that lie within the band gap [5-9], (b) 3D localization of light at point-defect sites [13,14], (c) threshold-less lasers [1,15], (d) 3D wave-guiding [10-12], (e) broadband omnidirectional reflectors [3,4,7], and (f) efficient solar cells [16,17]. In order to be widely usable, an ideal 3D photonic crystal should possess the following properties:

- A wide and complete band gap
- The ability to introduce controlled line and point defects
- Ease of fabrication, reproducibility and silicon-compatibility
- Large area manufacturability

Although several different approaches to fabricate 3D photonic crystals have been developed, it is still difficult to meet all four requirements simultaneously. First of all, only diamond and diamond-like structures are amenable to a complete band gap [14] and therefore, most experimental work to date revolves around fabrication of diamond-like 3D photonic crystals. Yablanovite was the first 3D crystal to be fabricated in a dielectric medium by drilling centimeter-sized holes along three face-centered-cubic (fcc) lattice vectors [18]. However, scaling down this crystal to optical frequencies and introducing controlled defects is extremely challenging [19]. 3D photonic crystals have also been fabricated using inverse-opals [20-21]. In this technique, a template is first created using close-packed, fcc-ordered colloidal spheres which is then infiltrated with high-index material such as Si using chemical vapor deposition. Finally, the template is removed, leaving behind air-sphere crystals in Si. As an alternative to opals, holographic lithography has also been used to create polymer-based templates [22]. These template-based techniques became quite popular because of the relative ease of fabrication, however the maximum width of the band gap remained narrow [23] and therefore sensitive to fabrication imperfections which are challenging to avoid [24]. In addition to large number of unintentional defects, it is also difficult to introduce controlled defect sites in this methodology.

Another diamond-like structure that offers a wide photonic band gap is the 3D woodpile photonic crystal which is fabricated by sequential stacking of layers of semiconductor logs. The Kyoto University group has been instrumental in the development and understanding of the woodpile photonic crystal made from III-V semiconductors and silicon using a wafer fusion technique with precise control over the alignment. Using their methodology, the group has successfully demonstrated wide 3D photonic band gaps [4], spontaneous emission control [5-7], three-dimensional waveguiding of photons [11,12], surface modes of 3D photonic crystals [25] and optical cavities [5,6]. The research group also developed another innovative technique for the fabrication of woodpile structures which used angled etching at $\pm 45^\circ$ to create two sets of mutually perpendicular logs [7]. These examples show that the

woodpile structure holds a great potential when it comes to the demonstration of interesting and unique properties of 3D photonic crystals. One limitation that has prohibited its widespread adoption is the advanced fabrication method that uses non-standard techniques only available in a few laboratories [26]. Additionally, large area manufacturability, such as on solar cells, is also questionable. Nevertheless, the woodpile structure, led by the Kyoto University group, has opened several new avenues to study and understand the 3D photonic crystal science.

In this work, we have demonstrated a complete photonic band gap using a slightly different class of 3D photonic crystals known as the inverse woodpile structure. As the name suggests, this structure consists of low-index logs or cylinders periodically embedded in a

high-index medium resulting in a wide band gap. This structure has been discussed in detail in the subsequent section. Specifically, the fabrication methodology developed in this work ensures that this structure possesses all the four important properties of an ideal 3D photonic crystal, discussed above, which have remained elusive and have hampered their widespread adoption. Using this methodology, we demonstrate a complete photonic band gap and hence a broadband omnidirectional reflector. This method also offers complete control on the placement of intentional line and point defect sites and therefore can be readily extended to form 3D waveguides and optical cavities.

3.2 THE INVERSE WOODPILE PHOTONIC CRYSTAL

The inverse woodpile is an extensively studied 3D photonic crystal. Its wide and complete photonic band gap [27], conceptual ease of fabrication [28,29], and robustness to disorders and fabrication imperfections [30] make it an ideal choice for building photonic crystals capable of providing ultimate control of light in all 3 dimensions. The basic structure of the inverse woodpile structure is illustrated in Fig. 1(a). It consists of two identical and mutually perpendicular sets of low-index cylinders embedded in a high-index medium. In this work, the set of cylinders aligned along the x-axis is referred to as the ‘out-of-plane’ set whereas that aligned along the z-axis is, hereafter, referred as the ‘in-plane’ set. The axis of the in-plane set is aligned exactly between the surrounding out-of-plane set cylinders, as evident from the cross-sectional schematic of the structure in Fig. 1(b). Each set is a centered-rectangular lattice with sides equal to ‘a’ and ‘c’. If the ratio of ‘a’ and ‘c’ equals $2^{0.5}$, the crystal symmetry becomes cubic and the structure is then diamond-like [27,28]. The band structure of such a photonic crystal is shown in Fig. 1(c). It is computed with the assumption that the ratio between the radius of the low-index cylinders ‘r’ and the lattice constant ‘a’ equals to 0.24 which is known to yield the largest band gap [27,28]. In this case, the gap to midgap ratio, $\Delta\omega/\omega_c$, is equal to 23.6%.

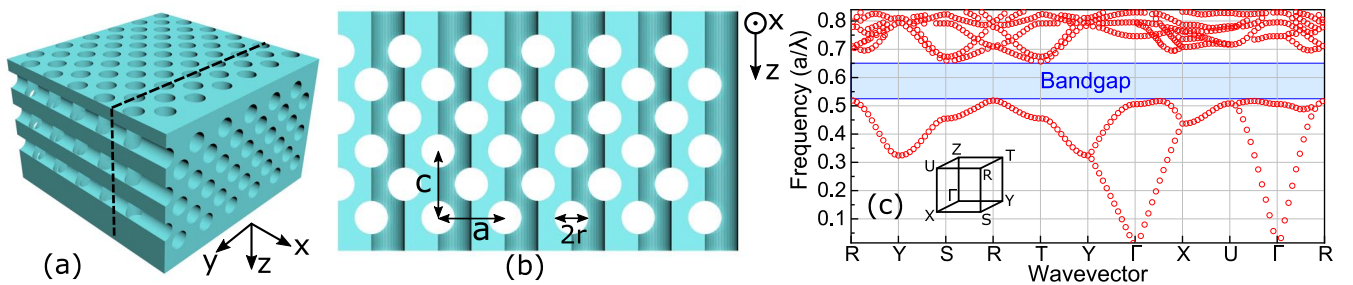


Figure 1: (a) Schematic of the inverse woodpile photonic crystal, (b) Cross-section cut of the inverse woodpile structure showing two mutually perpendicular sets of cylinders and the relevant design

parameters and (c) Band diagram of the photonic crystal assuming a/c is equal to $2^{0.5}$ and r/a equal to 0.245. The first Brillouin zone is also shown in the inset.

There have been multiple reports that experimentally demonstrate a complete band gap for the inverse woodpile structure. However, none of them uses a fabrication methodology that is truly Si compatible nor one that can be easily mass-produced by any standard semiconductor fabrication facility. Schilling et. al. demonstrated the first experimental inverse woodpile photonic crystal [31]. They first created a two-dimensional photonic crystal by etching deep pores into Si using wet etchants, creating ‘macroporous’ silicon. This structure was then cleaved and the second pore set was then drilled perpendicular to the first by using focused-ion-beam (FIB)-milling. Though this was the first Si-compatible demonstration of the inverse-woodpile structure, the cleaving and the subsequent FIB-milling make it prohibitive in terms of mass-production and repeatability. Moreover, FIB-milling the second set of pores makes it a time-consuming process and thus the scalability of this process to larger areas is poor. Such a photonic crystal has the potential to be the perfect back-reflector for solar cell applications [16] and therefore scalability to larger areas while keeping the cost down at the same time is important. In addition, it is difficult to introduce controlled defects in such a process flow and hence it is not well-suited for the fabrication of waveguides and cavities using the inverse woodpile structure. A similar approach has been adopted by the researchers from the University of Twente, who have also studied the inverse-woodpile structure theoretically [30,32,33] and experimentally [9,29,34]. Instead of using wet-etching techniques to make macroporous silicon, they use reactive-ion etching to obtain an array of deep pores. In the next step, the structure is cleaved and FIB-milled as was done by Schilling et. al. and therefore this process flow is also plagued by the same issues.

In the next section, a truly Si compatible method to fabricate the 3D inverse woodpile photonic crystal is shown. This method allows for a scalable mass-production of the photonic crystal as it uses a standard toolset available in most fabrication facilities.

33 FABRICATION METHODOLOGY

As discussed in the last section, the inverse woodpile structure consists of two identical and mutually perpendicular sets of cylinders - the out-of-plane set and the in-plane set. The in-plane set of cylinders can be readily made by reactive ion etching [9,29,34,35]. Fabricating the out-of-plane set in a way that is truly Si compatible is the main challenge. In this work, we present a novel solution to this challenge by means of a unit process called ‘empty-space-in-silicon’ (ESS) technique developed by Toshiba as an alternative to the silicon-on-insulator (SOI) substrate [36,37]. Using this technique, empty spaces of different shapes such as spheres, cylinders or plates can be buried inside a silicon substrate. The basis of this technique is the self-organizing re-crystallization of nanostructures due to surface migration of silicon. It was shown that a trench can be transformed to a spherical ESS when it is annealed in a reducing ambient, such as hydrogen. This reducing ambient, unlike oxidizing, allows the surface atoms to be mobile and hence minimize the surface energy. This process of surface migration has been successfully modeled using the Mullin’s surface diffusion equation [38,39]. Using the same equation, a 3D simulator was also developed to predict the shape transformation caused by silicon migration [40]. The time evolution of an isolated trench to a spherical ESS when annealed in a reducing ambient, is shown in Fig. 2(a). The simulator used is very similar to that in Ref. 40 and the time units shown in Fig. 2(a) correspond to those in simulations, not seconds. It is evident that the transformation begins at the top and bottom

of the trench because the radius of curvature of these regions is the smallest. The top opening of the trench eventually closes as surface migration continues to transform it into a spherical shape which

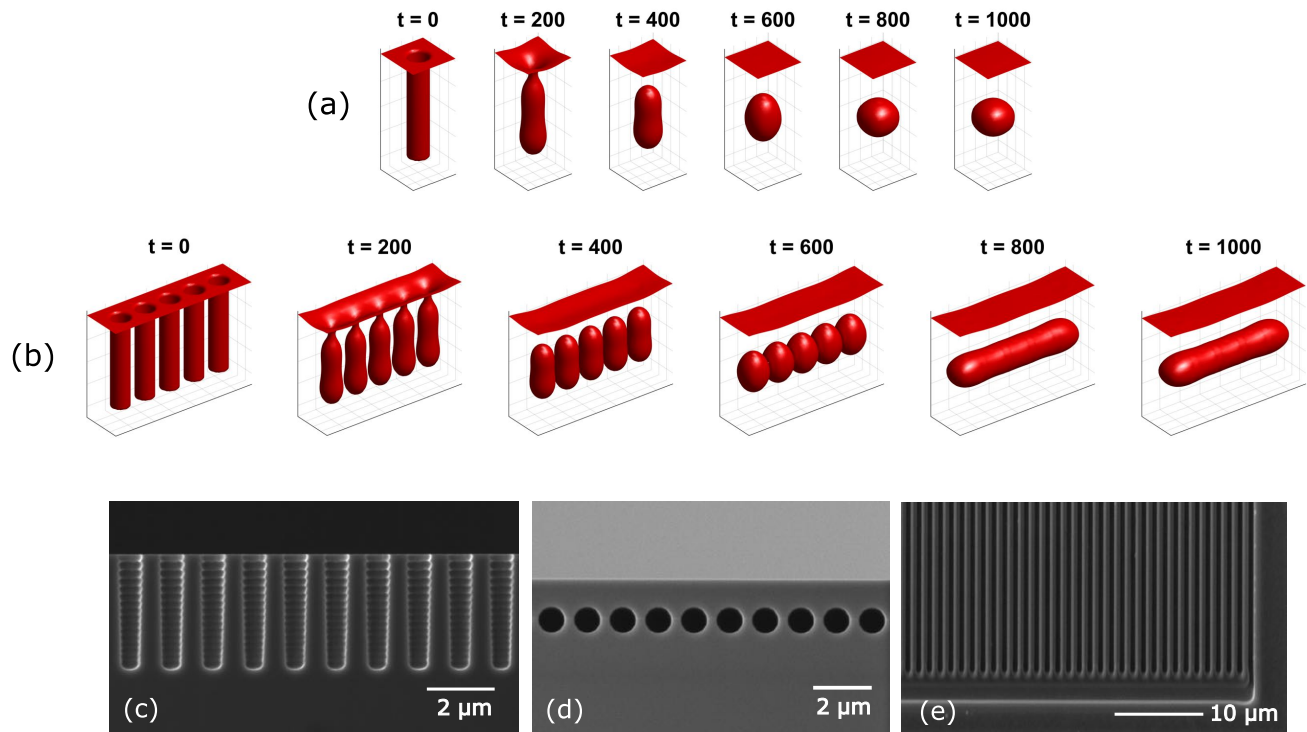


Figure 2: (a) Transformation of an isolated trench (in simulation time units) to a spherical empty-space-in-silicon (ESS) when annealed in a reducing ambient, (b) Evolution of trenches arranged closely in one dimension to a cylindrical ESS, (c) SEM image of trenches etched by using Bosch process, (d) Cross-section SEM of air-cylinders embedded in Si and (e) Top-view of the air-cylinders after etching away Si from top.

minimizes the overall surface energy. Once this minimum energy state is reached, further shape evolution ceases and the ESS becomes extremely stable. The shape and dimension of this ESS can be fully controlled by the dimensions of the initial trench^{36,37}. During this process, the Si mass is conserved and hence the volume of the initial trench and the final spherical ESS remains the same. This implies that the diameter of the spherical ESS becomes larger than the width of the initial trench which helps to form cylindrical ESS as shown in Fig. 2(b). In this case, trenches are arranged closed to each other in one dimension. When subjected to annealing in reducing ambient, the diameter of the subsequent ESS grow and eventually coalesce into each other, thereby forming a cylindrical ESS in the stable, minimum energy state. These cylindrical ESS can be readily used to make a layer of out-of-plane cylinders.

In this work, we have used the well-known Bosch process for reactive-ion etching of initial trenches in Si, as shown in Fig. 2(c). These trenches were then subjected to hydrogen anneal at 1150°C provided by an Applied Materials reduced-pressure chemical vapor deposition (CVD) system. The cross-section of the minimum energy state made up of air-cylinders embedded inside Si is shown in Fig. 2(d). A top-view obtained after etching the Si on top of the cylinders is shown in Fig. 2(e). Since these air-cylinders

are made after self-limited recrystallization of silicon, their surface roughness is extremely low and hence they make a perfect candidate for photonic crystal applications.

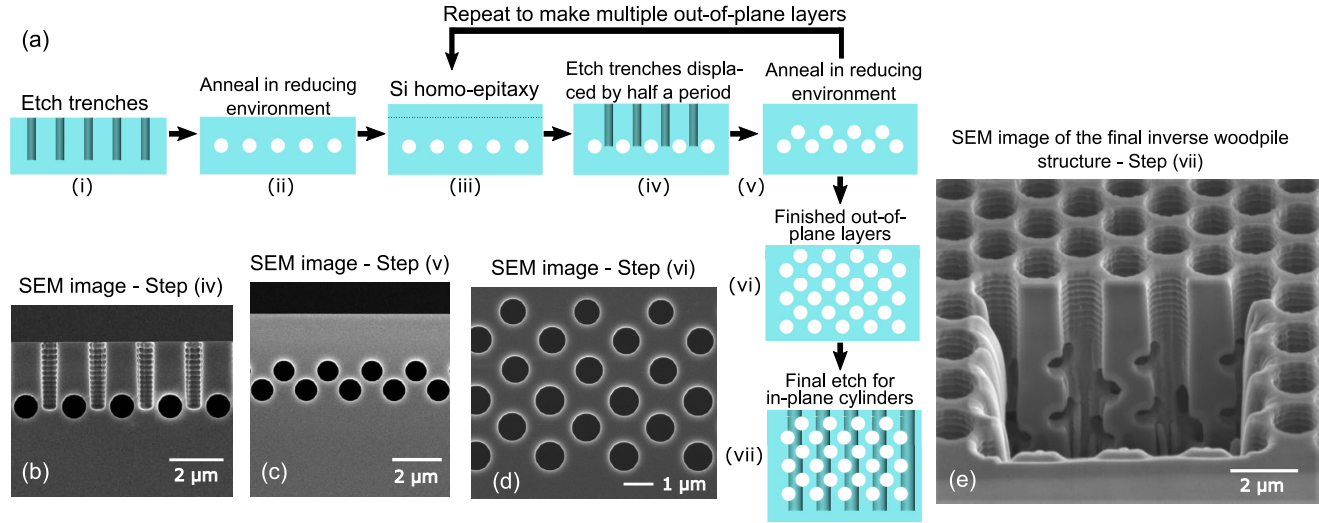


Figure 3: (a) Process steps for the fabrication of inverse woodpile photonic crystal, (b), (c), (d) SEM images corresponding to the process steps and (e) SEM image of final inverse woodpile structure.

The most attractive feature of this process is that the air-cylinders are extremely stable, once formed. This is due to the self-limiting nature of the minimum energy state. Any additional process steps and exposure to more thermal budgets do not perturb the cylinders at all. We have utilized this feature and stacked multiple layers of air-cylinders in a way that constitutes the out-of-plane set for the inverse woodpile structure. The process steps are outlined in Fig. 3a. After fabricating the first layer of air-cylinders, as outlined above, Si homo-epitaxy was done in the same Applied Materials CVD system without breaking vacuum. The Si epitaxial layer thickness was kept equal to half the vertical lattice constant ' c '. Next, trenches were etched in the middle of the air-cylinders formed for the first layer as shown in Fig. 3b. The trenches were displaced by half the lattice constant ' a ' in order to make the out-of-plane layer centered-rectangular, as discussed before. These trenches were then subjected to exactly the same anneal conditions as was done for the first layer. In this way, two layers of air cylinders were fabricated, as shown in Fig. 3c. The same process can be repeated to get a large number of layers arranged in a centered-rectangular lattice with parameters ' a ' and ' c '. Fig. 3d shows 4 such layers with lattice constant ' a ' equal to $2.5 \mu\text{m}$ and ' c ' equal to $2 \mu\text{m}$, in this proof-of-concept work. The radius ' r ' of the air-cylinders is kept at $0.5 \mu\text{m}$, thereby making r/a ratio equal to 0.2. The crystal parameters are limited by the critical dimension of the lithography system used. In this work, we have used the ASML PAS 5500/60 to define the trench patterns and kept the critical dimension to 600 nm to ensure good repeatability and excellent alignment of each layer on top of the other. The structure can be readily scaled to smaller dimensions through the use of more advanced optical lithography system or electron-beam lithography.

Once all the desired layers in the out-of-plane set are fabricated, the in-plane set can be easily made by simply etching trenches in a centered-rectangular lattice with exactly the same dimensions as that of the out-of-plane set. The in-plane set is also shifted by a quarter of the lattice constant ' a ' with respect to the out-of-plane set so that the vertical cylinders are placed in the middle of the surrounding horizontal cylinders. The final inverse woodpile structure with 4 layers in the out-of-plane set and the

final in-plane set is shown in Fig. 3e. In this proof-of-concept work, photonic crystals with 4 and 6 out-of-plane layers were fabricated. To our knowledge, this is the first demonstration of the inverse woodpile photonic crystal using truly Si compatible methods. The process developed requires repeated use of lithography, standard reactive-ion etching and annealing steps and all these tools are regularly available in a semiconductor fabrication facility.

This layer-by-layer process also allows complete control of intentional line and point defects which are necessary to extend this process for fabrication of waveguides and optical cavities. Theory shows that the line defects in the inverse woodpile structure can be formed by varying the radius of one or more air-cylinders embedded in Si and therefore the intersection of two such line defects, one in the in-plane set and one in the out-of-plane set, will constitute a point defect[32]. This process allows the radius of each individual air-cylinder, both for the in-plane and out-of-plane set, to be controlled independently making it is very well suited for the fabrication of 3D waveguides and optical cavities.

3.4 DEMONSTRATION OF AN OMNIDIRECTIONAL BROADBAND REFLECTOR

The structure discussed in the last section constitutes an inverse woodpile photonic crystal that can be readily used as an omnidirectional broadband reflector due to its large and complete band gap. In this demonstration, crystal lattice constant 'a' equals $2.5\ \mu\text{m}$, lattice constant 'c' equals $2\ \mu\text{m}$ and the radius 'r' of the air cylinder equals $0.5\ \mu\text{m}$. The reflectivity of this photonic crystal is measured using FTIR spectroscopy and is shown in Fig. 4(a) along with the band diagram computed for the same parameters as the experiments. The measurement is done for crystals with 4 and 6 out-of-plane layers. The reflectivity is measured with normal incidence in the z-direction and the infra-red source is kept un-polarized. For these parameters, a broad reflection peak is observed between $5.7\ \mu\text{m}$ and $6.7\ \mu\text{m}$ wavelength which coincides well with the band gap in the Γ -Z direction as shown in Fig. 4(a). Observation of reflection peaks alone is not sufficient to prove a band gap because such peaks can also arise when incident waves do not couple to a mode inside the crystal. However, the alignment of experimental reflection peaks with the stop gap in its band structure is a clear signature that the reflection from the photonic crystal is due to the absence of allowed states [33,41]. Moreover, reflectivity greater than 85% can be achieved with only 6 out-of-plane layers. For comparison, another sample with only in-plane set and no out-of-plane layer of cylinders was prepared and measured, as shown by the blue curve in Fig. 4(a). It is evident that the reflection peak is absent for this sample and the spectrum is modulated by Fabry-Perot fringes due to the finite depth of the trenches etched for the in-plane set. Similar Fabry-Perot fringes can be observed in the reflectivity spectrum of the full inverse woodpile structure as well.

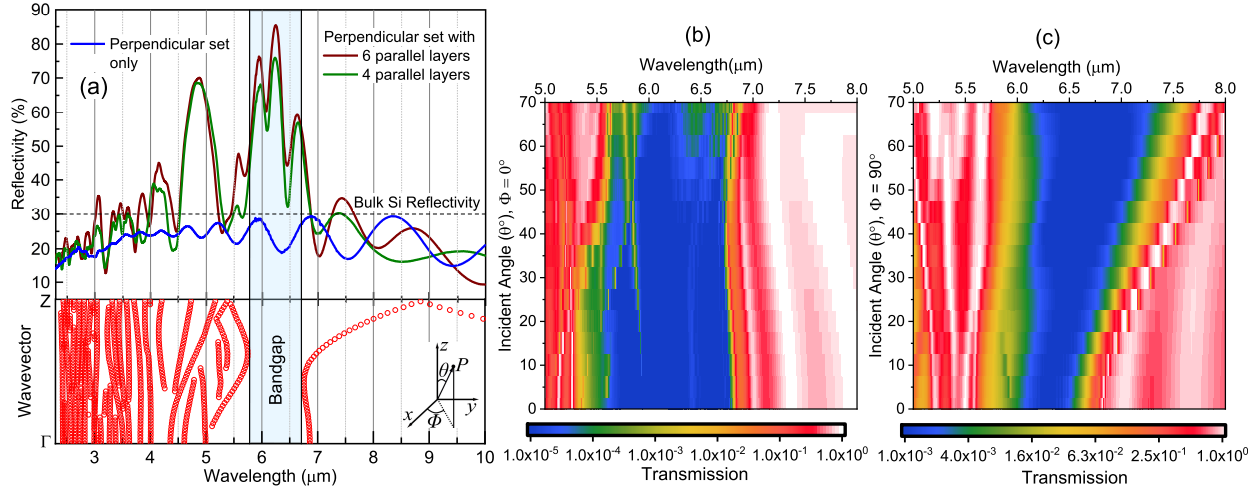


Figure 4: (a) Reflectivity measurements of the fabricated inverse woodpile photonic crystal (top) and the corresponding band diagram (bottom) with the co-ordinate system used (inset); Simulated transmission spectrum of the crystal as a function of polar angle of incidence (θ) with azimuthal angle (Φ) fixed at (b) 0° and (c) 90° .

This reflector is expected to be omnidirectional because of the complete band gap offered by the inverse woodpile structure. This is further confirmed by incident-angle resolved FDTD transmission simulations shown in Fig. 4(b) and (c). The light is incident at a fixed azimuthal angle (Φ) of 0° in Fig. 4(b) and 90° in Fig. 4(c) while the polar angle (θ) is varied from 0 to 70° . A broad transmission trough several orders of magnitude deep emerges in both cases. This proves that a complete band gap exists and the structure can indeed be used as an omnidirectional reflector. The transmission trough aligns well with the measured reflection peak and provides another proof that the measured reflection peak emerges because of the complete band gap of the fabricated inverse woodpile structure. Additionally, the Fabry-Perot fringes observed in the measured reflectivity spectrum can also be seen in the simulations, giving us ample confidence that the experiments are well explained by the FDTD simulations.

3.5 CONCLUSION

We have developed a truly Si-compatible process for the fabrication of inverse woodpile photonic crystals with a complete band gap. Using this process, we demonstrated a broad- band omnidirectional reflector on Si. The developed process leads to defect-free, stable, and high-quality crystals since it relies on self-limited recrystallization of Si atoms to an energy- minimum state. The different design parameters such as the lattice constants ‘a’ and ‘c’ and the radius ‘r’ of the air-cylinders are scalable and can be tailored to the needs of a given application. Moreover, the process allows for tuning of the radius ‘r’ of each air-cylinder individually, easily extending this method for the fabrication of 3D waveguides and optical cavities. The process can also be utilized for large-area fabrication of photonic crystals in applications such as solar cells etc. Finally, use of standard fabrication equipment ensures that this process can be widely adopted by research groups and industries alike and will help in making 3D photonic crystals a fundamental building block for the realization of ultimate control of photons in three dimensions.

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List of publications supported by this grant

Peer-reviewed journal publications

- [1] Youngmin Kim, Jan Petykiewicz, Shashank Gupta, Jelena Vuckovic, Krishna C. Saraswat, and Donguk Nam, "Strained Ge Light Emitter with Ge on Dual Insulators for Improved Thermal Conduction and Optical Insulation" *IEIE Trans. on Smart Processing and Computing*, Vol. 4, No. 5, p. 318-323, October 2015.
- [2] David S. Sukhdeo, Y. Kim, S. Gupta, K. C. Saraswat, B. Dutt and D. Nam, "Theoretical Modeling for the Interaction of Tin alloying with N-type Doping and Tensile Strain for GeSn Laser," *IEEE Elec. Dev. Lett.* Vol. 36, No. 8, August 2015, pp.1307 – 1310.
- [3] Ashwyn Srinivasan, M. Pantouvaki, S. Gupta, H. T. Chen, P. Verheyen, G. Lepage, G. Roelkens, K. Saraswat, D. V. Thourhout, P. Absil, and J. V. Campenhout, "6Gb/s Germanium Waveguide Electro-Absorption Modulator," *IEEE/OSA J. Lightwave Technol.*, Vol. 34, No. 2, pp. 419 - 424, January 15, 2016
- [4] J. Petykiewicz, D. Nam, D. Sukhdeo, S. Gupta, S. Buckley, A. Piggott, J. Vuckovic and K. Saraswat, "Direct Bandgap Light Emission from Strained Germanium Nanowires Coupled with High-Q Nanophotonic Cavities," *Nano Letters*, 2016; 16 (4): 2168-2173.
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- [7] Shashank Gupta, S. Tietz, J. Vuckovic, and K. Saraswat, "A new paradigm for silicon-compatible fabrication of inverse woodpile photonic crystals with a complete band gap," *ACS Photonics*, ACS Photonics, 2019, 6 (2), pp 368–373

Refereed conference publications

- [8] Shashank Gupta, J. Petykiewicz, D. Nam, D. Sukhdeo, J. Vuckovic and K. Saraswat, "Dramatic and previously overlooked interaction between strain and parasitic absorption in germanium with major implications for Si-compatible lasing," *CLEO:2016*, Paper # SW1M.4, San Jose, CA, June 2016.
- [9] Shashank Gupta, J. Petykiewicz, D. Nam, D. Sukhdeo, J. Vuckovic and K. Saraswat, "Remarkable interplay between strain and parasitic absorption unravelling the best route for Ge based Si-compatible lasing at room temperature," *IEEE Photonics Conf.*, pp. 88-89, Waikoloa, Hawaii, October 2016.

Invited conference presentations

- [10] Krishna Saraswat, "Real Limits to Nanoelectronics: Interconnects and Contacts," *International Electron Devices & Materials Symposium (IEDMS 2017)*, Hsinchu, Taiwan, Sept. 2017, (Keynote).
- [11] Krishna Saraswat, "Emerging Interconnect Technologies for Nanoelectronics," *NanoWorld Conf.* San Francisco, April 2018. (Keynote)
- [12] Krishna Saraswat, "Emerging Interconnect Technologies for Nanoelectronics," *IEEE VLSI Symp.*, June 2019, Kyoto. (invited).

Scientific Personnel Supported by This Project

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