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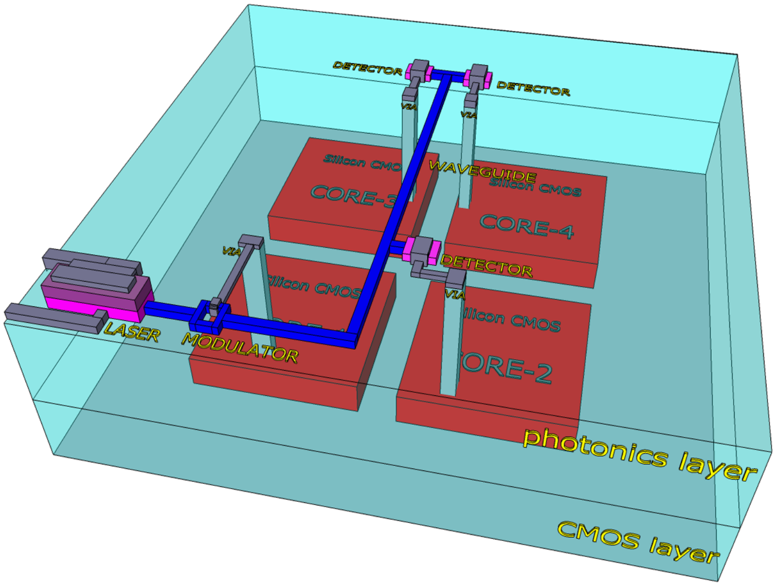
Birendra (Raj) Dutt, Member, IEEE
Devanand S. Sukhdeo, Student Member, IEEE
Donguk Nam, Student Member, IEEE
Boris M. Vulovic
Ze Yuan, Student Member, IEEE
Krishna C. Saraswat, Fellow, IEEE



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Roadmap to an Efficient Germanium-on-Silicon Laser: Strain vs. n-Type Doping

Birendra (Raj) Dutt,[1,2] ***Member, IEEE,***
Devanand S. Sukhdeo,[1,3] ***Student Member, IEEE,***
Donguk Nam,[3] ***Student Member, IEEE*****, Boris M. Vulovic,**[1]
Ze Yuan,[3] ***Student Member, IEEE*****, and Krishna C. Saraswat,**[3] ***Fellow, IEEE***

[1]APIC Corporation, Culver City, CA 90230, USA
[2]PhotonIC Corporation, Culver City, CA 90230, USA
[3]Department of Electrical Engineering, Stanford University, Stanford, CA 94305, USA

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Abstract: We provide a theoretical analysis of the relative merits of tensile strain and n-type doping as approaches to realizing an efficient low-power germanium laser. Ultimately, tensile strain offers threshold reductions of over 200x, and significant improvements in slope efficiency compared with the recently demonstrated 0.25% strained electrically pumped germanium laser. In contrast, doping offers fundamentally limited benefits, and too much doping is harmful. Moreover, we predict that tensile strain reduces the optimal doping value and that experimentally demonstrated doping has already reached its fundamental limit. We therefore theoretically show large ($>$ 1%) tensile strain to be the most viable path to a practical germanium-on-silicon laser.

Index Terms: Semiconductor lasers, diode lasers, semiconductor materials, optoelectronic materials, infrared lasers, theory and design.

1. Introduction

Germanium (Ge) has emerged as a leading contender for silicon (Si) compatible optical interconnects due to advances in Ge-on-Si heteroepitaxy [1]. Researchers have demonstrated Ge modulators [2] and detectors [1] integrated directly on Si, but an efficient Ge light source remains elusive due to Ge's indirect band gap. Researchers have proposed to overcome this limitation by employing heavy n-type doping [3], [4] and/or applying tensile strain [3], [5]. By employing heavy doping in conjunction with a small biaxial tensile strain, researchers from MIT and APIC Corporation have recently demonstrated an electrically pumped Ge-on-Si laser [6]. However, this laser suffered from both an extremely high threshold ($\sim$280 kA/cm^2) and very poor efficiency, since only $\sim$1 mW of output was observed despite the enormous $\sim$350 kA/cm^2 current driven into a 172-μm waveguide [6]. Such a device cannot be practical without both a drastic reduction in the threshold and a vastly improved efficiency. It is therefore worthwhile to quantitatively compare the relative merits of tensile strain and n-type doping in the pursuit of an efficient low-threshold Ge laser. For the purposes of this analysis, all strains are biaxial tensile.

2. Qualitative Analysis

The fundamental roadblock with Ge lasers is the presence of the indirect L-valley in the conduction band, which is not only slightly lower in energy than the direct Γ-valley but also has a much higher density of states. Thus, only $\sim$0.01% of electrons will reside in the Γ-valley for unstrained Ge, and an extraordinarily large number of electrons are required to achieve population inversion across the direct band gap. This high carrier density degrades laser performance by introducing large amounts of free carrier absorption (FCA) and recombination, particularly Auger recombination, thus degrading both threshold and efficiency.

One proposed solution is n-type doping. Because of the indirect L-valley, an enormous number of electrons are needed for population inversion, but assuming equal carrier injection, a very large number of unneeded holes will also be injected. By employing n-type doping, extrinsic electrons can be added to the active region without adding unwanted holes, eliminating these holes' contribution to recombination and FCA. However, there will be an optimal doping value where all the desired extrinsic electrons have been added; adding even more extrinsic electrons would then only result in more recombination and more FCA from electrons.

The other approach considered for improving Ge laser performance is band engineering via tensile strain. Biaxial strain lowers the direct valley faster than the indirect valley, and it is generally believed that 1.7%–2.5% biaxial tensile strain will turn Ge into a direct band-gap material [7]–[10]. Applying tensile strain thus allows population inversion to be achieved with reduced hole densities and reduced electrons densities, with emission at longer wavelengths. Researchers have demonstrated that straining Ge photodetectors extends their detection range to correspondingly longer wavelengths [11], strongly implying that a chip-scale Ge optical link can operate at these longer wavelengths, although long-distance telecommunications applications may be more problematic.

3. Quantitative Analysis—Threshold

To quantify the Ge laser performance, the threshold current of a double-heterostructure Si/Ge/Si laser is considered as a function of biaxial tensile strain and doping $(\mathrm{N_d})$. We have used an $sp^3d^5s^*$ tight-binding model [12], [13] to calculate the band structure of strained Ge and then computed the quasi-Fermi levels versus carrier populations. Our model errs conservatively regarding strain by assuming a crossover of the direct band gap at 2.5% biaxial tensile strain. By extrapolating the absorption coefficient of [5] to higher strain values, along with the FCA equation and recombination coefficients [14]–[17] previously used in [5], the net gain spectrum in a slab of Ge can be computed as a function of current. As soon as the net gain matches the optical cavity loss, the gain clamps and lasing begins. By always considering only the wavelength of maximum net gain, the threshold for a Si/Ge/Si double heterostructure laser can be computed as a function of the strain and the doping. For a Fabry–Perot laser, this optical cavity loss is $\alpha_{cavity} = -\ln(R_1 R_2)/2L$. However, using only the more abstract α_{cavity} ensures that the conclusions of this analysis will be applicable not only to arbitrary facet conditions but also to arbitrary cavity designs such as ring resonators and microdisks.

For the analysis in this paper, the active region thickness is consistently taken to be 300 nm, in line with that of the experimental Ge laser [6]. But the thickness has no impact on the results except to scale all threshold current values by a constant factor assuming a constant optical confinement factor (Γ), which we have always taken to be $\Gamma = 1$. With these considerations in mind, the threshold current was mapped out as a function of strain and doping, as shown in Fig. 1 for a zero-loss optical cavity. This lossless (infinite Q-factor) cavity represents the cavity design that minimizes the threshold.

As shown in Fig. 1, there exists some optimal doping value for any given strain, a phenomenon very briefly alluded to in [18]. This optimum exists because eventually enough extrinsic electrons have been added to make up the difference between the desired electron and hole concentrations, and so, adding even more electrons only introduces more FCA and recombination. For example, at 0.5% strain and a lossless cavity, the threshold current goes from 130 kA/cm^2 to 8 kA/cm^2 as the doping is increased from $\mathrm{N_d} = 1 \times 10^{19}$ cm^{-3} to $\mathrm{N_d} = 1 \times 10^{20}$ cm^{-3}, but then increases to

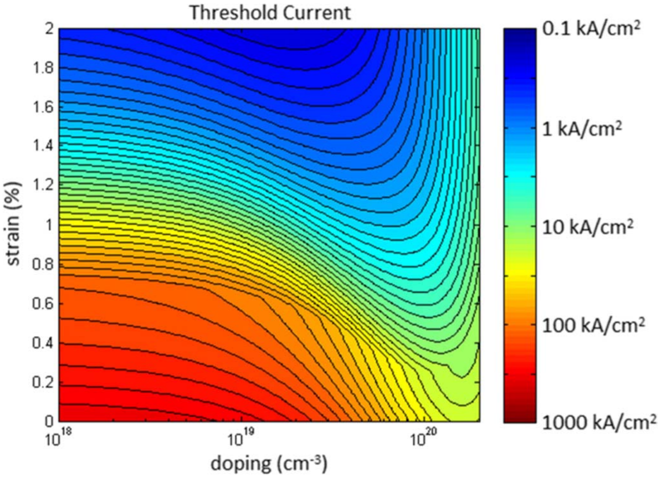
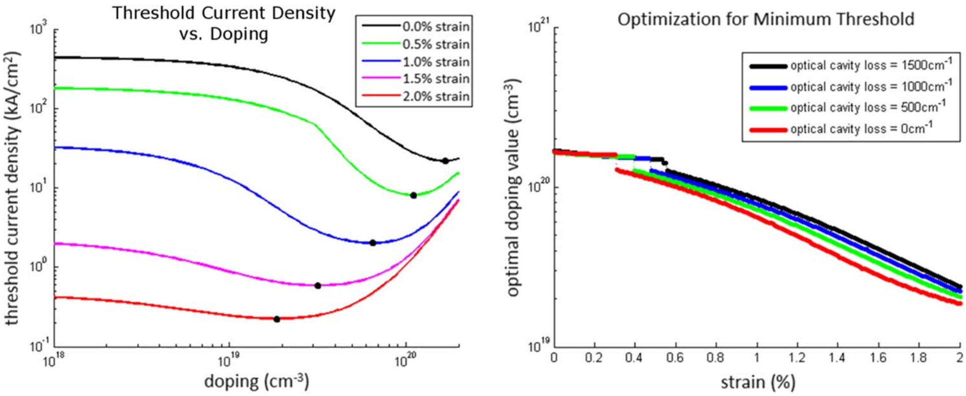


Fig. 1. Threshold current as a function of biaxial tensile strain and n-type doping, assuming a lossless (optical cavity loss $= 0$) cavity lasing at the wavelength of peak net gain.



(a) (b)

Fig. 2. (a) Threshold current versus doping for various strain values, showing that an optimal doping value (black dot) always exists. (b) Optimized doping value (for minimum threshold) versus strain.

15 kA/cm^2 as the doping increases to $N_d = 2 \times 10^{20}$ cm^{-3}. This effect is clearly illustrated in Fig. 2(a). Moreover, because tensile strain reduces the difference between the Γ- and L-valleys, fewer states in the L-valley need to be "filled up" by doping when large strains are employed. As a result, the threshold-optimized doping moves to a lower value as the strain increases, as shown in Fig. 2(b). This means that very highly strained Ge lasers would require the doping to be reduced from current levels. For example, starting from 0.25% strain and $N_d = 5 \times 10^{19}$ cm^{-3}, increasing the strain to 2.0% can reduce the threshold by more than 200x, but only if the doping is then reduced to $N_d \approx 2 \times 10^{19}$ cm^{-3}.

Notably, at 1.1% strain, the optimal doping is only 5.7×10^{19} cm^{-3}. Since 1.1% biaxial tensile strain has been experimentally demonstrated in suspended Ge membranes on Si substrates using external stressors [11], and since an implant-free n-type active dopant concentration of $\sim 5 \times 10^{19}$ cm^{-3} has already been claimed [19], it would appear that researchers have already pushed doping to its fundamental limit if this 1.1% strain can be applied to a Ge laser. Using harsher implant-based approaches such as codoping of phosphorus and antimony [20] or laser annealing [21], researchers have pushed the n-type doping beyond 1×10^{20} cm^{-3} and 2×10^{20} cm^{-3}, respectively, exceeding the optimal value for even unstrained Ge. More importantly, since biaxial tensile strains of 2.00% and 2.33% have been demonstrated in Ge using gas pressure [22] or

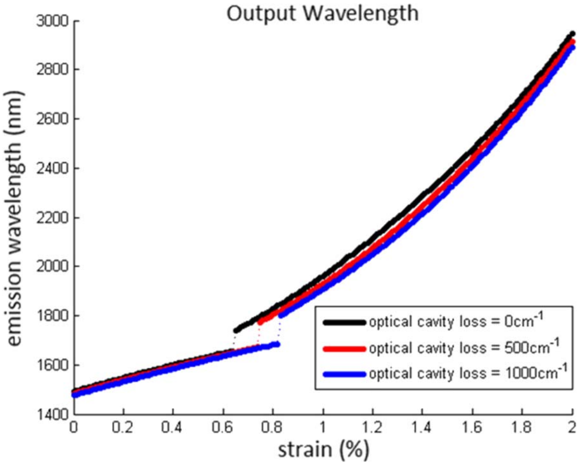


Fig. 3. Emission wavelength versus strain for various modal losses in the optical cavity, assuming 1×10^{19} cm^{-3} n-type doping.

growth on a relaxed InGaAs/GaAs buffer [23], respectively, the mechanical limit of strain in Ge has clearly not yet been reached, and several strain approaches are under active investigation [11], [24]–[28]. As researchers achieve CMOS-compatible strains beyond 1.1% in Ge-on-Si, the optimal doping will continue to decrease exponentially, and so, it will become necessary to actually reduce the doping below 5×10^{19} cm^{-3} in order to achieve the best performance.

Another feature is that a kink or discontinuity generally appears as the strain exceeds approximately ~0.6%. This is because the top of the light-hole (LH) band rises above the heavy-hole (HH) band under biaxial strain. For low strains, population inversion into the HH band is required to overcome free carrier losses; however, for a large LH/HH splitting, lasing becomes possible from the top of the LH band alone. An abrupt shift emission wavelength thus appears as the strain exceeds ~0.6%, as shown in Fig. 3. Similar features will also appear in later figures due to this phenomenon. This also shows the importance of rigorously finding the wavelength most likely to laser for every different combination of strain, doping (not shown below), and optical cavity loss when modeling the Ge laser.

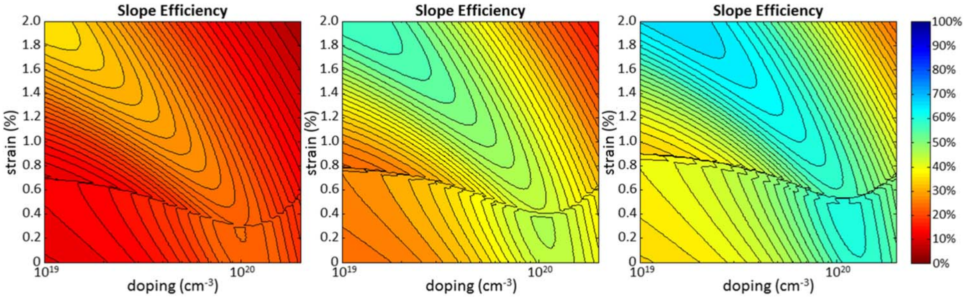
4. Quantitative Analysis—Slope Efficiency

Another key concern is the slope efficiency of an ideal Ge laser, which is determined by the ratio of the emitted photon energy to the injected electron energy and the fraction of photons emitted out the cavity rather than lost to FCA. The slope efficiency is therefore given by

$$\eta_{slope} = \left(\frac{E_{photon}}{qV_{bias}}\right)\left(\frac{\alpha_{cavity}}{\alpha_{cavity} + \alpha_{FCA}}\right)$$

assuming that α_{cavity} consists only of "loss" from photons exiting the cavity as useful emission. The bias voltage was determined from the quasi-Fermi level separation in the Ge active region, i.e., $qV_{bias} \approx E_{fn} - E_{fp}$. For the specific case of a Fabry–Perot cavity of length L with a perfectly reflective rear fact and a front facet of reflectivity R, the optical cavity loss will be given by $\alpha_{cavity} = -\ln(R)/2L$. Again, working only with the more abstract optical cavity loss allows this analysis to be directly applied to arbitrary facets and arbitrary cavity structures such as microdisks and ring resonators. The slope efficiency can thus be mapped out just like the threshold, as shown in Fig. 4. This slope efficiency is an upper bound since all parasitics, such as electrical and optical losses in the contacts, have been neglected.

The fact that lossy cavities are needed for acceptable slope efficiency has important implications that will be discussed shortly. More crucially, for any given strain value, there will be an optimal



Optical Cavity Loss = 250cm^{-1} *Optical Cavity Loss = 750cm^{-1}* *Optical Cavity Loss = 1500cm^{-1}*

Fig. 4. Slope efficiency of a Ge laser as a function of biaxial tensile strain and doping for various resonator conditions.

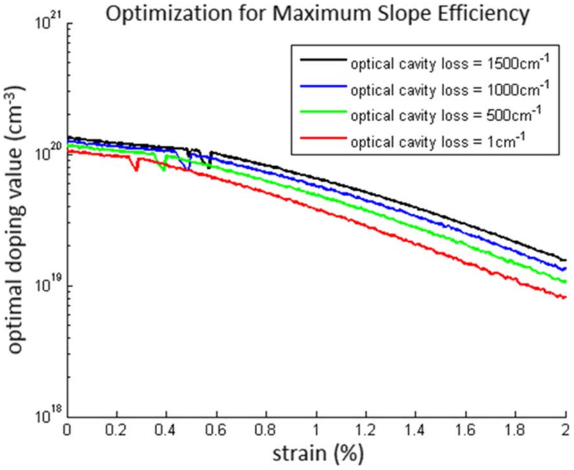
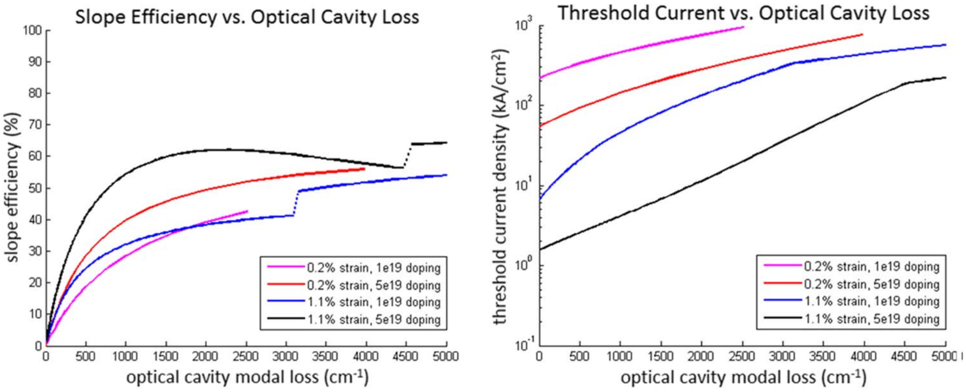


Fig. 5. Optimized doping value versus strain for various cavity losses. Doping is optimized for maximum slope efficiency.

doping beyond which the slope efficiency will worsen. The optimal doping for slope efficiency, shown in Fig. 5, follows a similar trend as the optimal doping for threshold, decreasing with strain, and increasing with optical cavity loss. Considering the case of 1.1% strain again, the optimal doping for slope efficiency is 3.3×10^{19} cm^{-3}–5.8×10^{19} cm^{-3} for an optical cavity loss of 0 cm^{-1}–1500 cm^{-1}. For threshold minimization, the optimal doping at 1.1% strain is 5.7×10^{19} cm^{-3}–7.6×10^{19} cm^{-3} for an optical cavity loss of 0 cm^{-1}–1500 cm^{-1}. Heavy doping beyond 5×10^{19} cm^{-3} is therefore even less desirable for slope efficiency.

By adjusting the cavity's modal loss there is an inevitable tradeoff between low threshold and high slope efficiency, as shown in Fig. 6. Because of the enormous carrier concentrations needed to achieve net gain in spite of the indirect band gap, the slope efficiency in Ge lasers is very strongly limited by the large FCA in the Ge active region itself. As such, an unusually large optical cavity loss will be required to achieve an acceptable slope efficiency, although this will inevitably come at the expense of threshold current.

There is a discontinuity in Fig. 6(a) for the 1.1% strain curves, which again corresponds to the LH/HH splitting. More importantly, from Fig. 6, it appears necessary to tolerate a 2–5x increase in threshold in order to achieve reasonable slope efficiency by introducing ~1000 cm^{-1} loss into the cavity. Low-loss cavities are therefore not viable for reducing the lasing threshold, intensifying the need for drastic threshold reductions by other means.



(a) (b)

Fig. 6. (a) Slope efficiency versus optical cavity loss. (b) Threshold current versus optical cavity loss assuming a 300-nm-thick Ge active region.

5. Comparison with Experimental Data

Finally, to test our model, we compare our predictions to the experimental data of the electrically pumped Ge laser under 0.25% strain with 4×10^{19} cm^{-3} n-type doping with a 300-nm-thick active region. Using these parameters, our model predicts a threshold current density of 76 kA/cm^2–174 kA/cm^2 for required material gains in the claimed range [29] of roughly 100 cm^{-1}–1000 cm^{-1}. This differs from the experimental value [29] of 280 kA/cm^2 by a factor of $\sim$3. Given the enormous parasitic effects, which our model ignores, such as high temperatures and leakage paths created by such extreme currents, this discrepancy is understandable. And so, our model is at minimum sufficiently valid to describe trends as in this letter. A validation for slope efficiency is not possible since insufficient information is publicly available and also because parasitic optical absorption in the metal contacts was a dominant factor [29].

Another interesting experiment is that of Carroll *et al.* [30], who were unable to observe optical amplification in Ge despite enormous pumping. Carroll *et al.* conclude that using only the FCA equation of Liu *et al.* [5], as we do here, neglects a significant absorption mechanism, transitions of free holes between the heavy-hole and split-off hole valence bands, and that this mechanism is responsible for a "pump-induced absorption" (PIA) in excess of any gain from the direct transition [30]. However, further analysis validates the FCA equation of Liu *et al.* [5], and this FCA and PIA as defined by Liu and Carroll, respectively, are in fact the same thing: both refer to intraband absorption from electrons and holes regardless of mechanism. We will further show that Carroll's observed "PIA" (same as FCA) is in at least marginal agreement in Liu's predicted "FCA" (same as PIA). The FCA equation of Liu [5] is an empirical fit to experimental data from Newman and Tyler [31] on absorption in heavily p-doped Ge. Not only must an empirical fit to experiments naturally incorporate all theoretical absorption mechanisms, but Carroll *et al.* also validated their experiments by claiming agreement with the results of Newman and Tyler [31], the same data set to which the FCA equation of Liu *et al.* [5] was fit. Ultimately, at 0.8 eV photon energy, Carroll *et al.* observe a PIA of $\sim$380 cm^{-1} per 10^{19} cm^{-3} holes at 400 K, which contrasts with the $\sim$180 cm^{-1} per 10^{19} cm^{-3} modeled by Liu *et al.* and observed by Newman and Tyler at 300 K for Ge with doping in the range of $10^{19}-10^{20}$ cm^{-3}. It is unclear how much of this discrepancy is due to the 100-K temperature difference. However, there is plainly no basis for Carroll's claim [30] that the theoretical model of Liu [5] is incomplete, and we have therefore used Liu's FCA equation [5], which is valid at 300 K. In addition, our calculations predict that increasing the FCA/PIA to a level more in line with Carroll's observations [30] will leave all general trends intact, and the optimal doping value itself would remain nearly unchanged. (Note that Carroll's criticism does apply to any theory that models the FCA/PIA using the Drude–Lorentz equation, e.g., [32].)

There is still a contradiction between our present theory and the inability to observe optical amplification in Ge of Carroll *et al.* [30]. The central disagreement here is in the gain from the direct transition *before* subtracting PIA/FCA. From Fig. 4(a) of Carroll *et al.* [30] we extract differential gains of 30–100 cm^{-1} per 10^{19} cm^{-3} injected carriers in Ge, which is less than one tenth the differential gain predicted by our theory and by that of Liu *et al.* [5]. This is surprising since the gain is simply the absorption coefficient times the population inversion factor; we used an absorption coefficient that was also fit to experimental data [5], and our tight-binding model yields effective masses and band energies in good agreement with accepted values. Moreover, like the model of Liu *et al.* [5], our model clearly explains the independent observations of optical amplification in Ge [33], [34] and subsequent device demonstrations [29], [35]. It remains to be seen why Carroll *et al.* [30] could not replicate the aforementioned results and thus contradict our predictions, but our theory is supported by a clear majority of relevant experiments to date [29], [33]–[35].

6. Conclusion

While heavy n-type doping has been key to recent breakthroughs of an electrically pumped Ge laser, further increases in the dopant concentration are not expected to yield the improvements needed to make this laser feasible. Strain, in contrast, offers threshold reductions of more than two orders of magnitude for biaxial tensile strains approaching 2.0%. For large tensile strains, it will be necessary to actually reduce the doping from its current value for the best threshold and slope efficiency. In addition, low-loss cavities are not a feasible path to a low-threshold laser, as very lossy optical cavities $(\sim 1000\ \text{cm}^{-1})$ will be needed for acceptable slope efficiency.

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