Impact of minority carrier lifetime on the performance of strained germanium light sources

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Abstract

We theoretically investigate the impact of the defect-limited carrier lifetime on the performance of germanium (Ge) light sources. For Ge LEDs, we show that improving the material quality can offer even greater enhancements than techniques such as tensile strain, the leading approach for enhancing Ge light emission. For Ge lasers, we show that the defect-limited lifetime becomes increasingly important as tensile strain is introduced, and that defect-limited lifetime must be improved if the full benefits of strain are to be realized. We conversely show that improving the material quality supersedes much of the utility of n-type doping for Ge lasers.

Keywords

Germanium; Optical Interconnects; Laser; LED; SRH lifetime; Strain

Germanium (Ge) light sources have garnered much attention for applications in both optical interconnects [1,2] and ultra-compact infrared sensing [3–5] due to Ge’s inherent CMOS compatibility. Techniques such as tensile strain and n-type doping have been proposed to enhance the performance of Ge light emitters and extensive modeling exists for these approaches [6–9]. The importance of material quality, however, has been generally overlooked. This is a serious gap in the literature: epitaxial Ge typically suffers from high defect densities and poor carrier lifetimes [10–12], a problem which is well known to inhibit efficient light emission. Moreover, it is important for experimentalists to know whether or not this low carrier lifetime will present a performance bottleneck as Ge light sources mature and, if so, how severe this bottleneck will be. To address these questions, we will theoretically investigate the impact of the defect-limited carrier lifetime on the performance of strained Ge LEDs and lasers. Through our theoretical modeling, we will show that improving the material quality is as important as band engineering in order to achieve efficient Ge LEDs. For Ge lasers, we will show that the defect-limited lifetime is an increasingly critical factor as tensile strain is introduced, and that this defect-limited lifetime must be improved if the full benefits of strain are to be realized. On the other hand, we will show that improving the material quality makes n-type doping a less useful technique for Ge lasers.

Our theoretical modeling process consists of various steps including: full bandstructure calculation, carrier statistics modeling, LED modeling, and laser modeling. The first step is to compute the full bandstructure of strained Ge over the intended range of strain values using $sp^3d^5s^*$ tight-binding following the approach of Refs. 13 and 14. As illustrated in Fig. 1, the use of tight-binding allows us to compute not just the bandstructures’ 2D cross sections (Fig. 1(a)) but also energies over a full $200 \times 200 \times 200$ mesh of k-points encompassing the entirety of the first Brillouin Zone (Fig. 1(b)). This gives the full 4D bandstructure, i.e. energy as a function of the three wavevector components k_x , k_y and k_z . Using our bandstructure model, we can also study general carrier statistics. To do this, we compute the occupancy probability given by Fermi-Dirac statistics for each allowed k-point and then integrate over the full k-point mesh of allowed energies encompassing the first Brillouin Zone to obtain the carrier concentration in each valley.

Based on the bandstructure model and carrier statistics, it is possible to model the

performance of a simple Ge LED. For this modeling, we will focus on the internal quantum efficiency (IQE) of a hypothetical Ge LED. Assuming a heterostructure design such that diffusion current is negligible and the injection efficiency will be virtually 100%, which can be achieved even in a simple Si/Ge/Si double heterostructure LED [15], the IQE will simply be the fraction of carrier recombination which is radiative. We can compute the radiative recombination rate using the following equation.

$$\begin{aligned} U_{\text{radiative}} &= R_L n_L p + R_\Gamma n_\Gamma p = R_L (n - n_\Gamma) p + R_\Gamma n_\Gamma p \\ &= R_L np + (R_\Gamma - R_L) n_\Gamma p = R_L np + (R_\Gamma - R_L) np \left(\frac{n_\Gamma}{n} \right) \end{aligned} \quad (1)$$

R_L and R_Γ are the recombination coefficients for indirect and direct recombination, respectively. n_L and n_Γ are the electron density in the indirect and direct conduction valley, respectively. n and p are the total electron and hole density, respectively. $\left(\frac{n_\Gamma}{n} \right)$ is the fraction of electrons in the direct conduction valley. The non-radiative recombination rate can also be computed using the following equation.

$$U_{\text{non-radiative}} = C_{\text{nnp}} n (np - n_i^2) + C_{\text{ppn}} p (np - n_i^2) + p / \tau_{\text{SRH}} \quad (2)$$

C_{nnp} and C_{ppn} are the recombination coefficients for nnp and ppn Auger process, respectively. n_i is the intrinsic carrier density. τ_{SRH} is the defect-limited carrier lifetime. The radiative recombination rate considers spontaneous emission from both the direct and indirect conduction valleys. Because of the much faster radiative recombination rate of the direct bandgap and also due to the increase of the $\left(\frac{n_\Gamma}{n} \right)$ term with strain, the total radiative recombination rate can be increased with strain significantly. The non-radiative recombination rate, meanwhile, does not depend on whether electrons are in the direct or indirect conduction valley and is therefore independent of strain. Then, finally, the IQE is simply the ratio of radiative recombination to total recombination as given in the following equation.

$$\text{IQE} = \frac{U_{\text{radiative}}}{U_{\text{radiative}} + U_{\text{non-radiative}}} \quad (3)$$

We can consider how the material quality affects the performance of double-heterostructure Ge LEDs, since the defect-limited carrier lifetime, τ_{SRH} , is a strong function of material quality [16]. In our modeling, we assume that the doping level is $1 \times 10^{19} \text{ cm}^{-3}$. As shown in Fig. 2, there is no conceivable level of strain that will result in an

efficient Ge LED if τ_{SRH} is less than 1 ns. On the other hand, if τ_{SRH} can be greater than 10 ns, the IQE can be greater than 50% for large strain values. Given that epitaxially-grown Ge films tend to have τ_{SRH} of approximately 1 ns [10,11], considerably less than the bulk lifetime values of >100 ns for the similar level of n-type doping [17], there is an acute need for research efforts such as those of Refs. 10–12,18 and 19 which explore innovative ways of improving the material quality and thereby improving τ_{SRH} . Without such efforts, an efficient CMOS-compatible LED is not possible no matter how much research efforts would be put into strain engineering and other techniques.

The penultimate goal of using band-engineered Ge is to build a low-threshold Ge-on-silicon laser for use in on-chip optical interconnects [20]. Prior modeling has answered some critical questions such as the relative merits of tensile strain and n-type doping [6], the impact of quantum wells [21,22] and the ideal crystal orientation [23], however the importance of material quality for a low-threshold Ge laser has hitherto been mostly overlooked. To finally investigate the importance of material quality, we extend upon our previous theoretical work [6] by singling out τ_{SRH} for careful investigation. Our laser modeling in this work employs the same approach explained in detail in our previous work [6] with one exception: we have used a corrected absorption coefficient [24] which better accounts for the splitting of the valence bands under biaxial tensile strain.

In the previous section, we showed that maximizing τ_{SRH} , presumably through improved material quality [11], is critically important to the performance of a Ge LED. Unsurprisingly, we find that maximizing the τ_{SRH} is also very important to achieving a low-threshold Ge laser. As shown in Fig. 3, there is no combination of strain and doping that gives a useable threshold for the case of a defect-limited carrier lifetime below 1 ns. On the other hand, improving τ_{SRH} to 100 ns makes it possible to achieve thresholds as low as 100 A/cm^3 . These benefits appear to start saturating once τ_{SRH} reaches about 100 ns. Given that most epitaxial Ge today has a lifetime of only about 1 ns, this means that it is absolutely imperative to improve the material quality if an efficient Ge laser is ever to be realized. Fortunately, this should be within the realm of possibility given that the bulk lifetime of Ge exceeds 100 ns [17]. Using nanoscale interfacial engineering, the minority carrier lifetime of Ge directly grown on Si has been already improved up to 9.3 ns [12]. It is also possible to further improve the minority carrier lifetime of Ge via wafer bonding followed by

chemical-mechanical polishing [11]. The minority carrier lifetime of >10 ns will allow us to achieve a lasing threshold of <10 kA/cm³ when combined with $\sim 1.9\%$ biaxial tensile strain [25] and 4×10^{19} cm⁻³ [26] while it is not possible to achieve such a low lasing threshold for the minority carrier lifetime of 1 ns regardless of strain and doping.

Due to the strain-induced bandgap narrowing, we observe a large redshift in the emission wavelength with strain as shown in Fig. 4. With 3.0% strain, the emission wavelength is redshifted from 1550 nm to nearly 5000 nm. Although the 1550 nm emission wavelength is important because it corresponds to the C-band minimum loss window for long-distance transmission on erbium-doped fiber, this is not particularly critical for short-distance chip-level optical interconnects since there exist waveguides and short-range optical fibers with reasonable transparency in these wavelength ranges [5]. Moreover, if a Ge light emitter can be strained to redshift its emission wavelength then a Ge modulator or photodetector can also be strained to similarly redshift its operating wavelength, and highly strained Ge photodetectors with a redshifted detection cutoff have already been demonstrated [27]. More interestingly, the ability to create light sources with the emission wavelength beyond 2000 nm allows us to create integrated mid-infrared sensors that have recently been attracting more attention [5].

Another interesting observation from our laser modeling is that improving τ_{SRH} appears to offer the most benefit for strain and doping combinations that give the smallest threshold. This is shown explicitly in Fig. 5(a) by plotting the threshold versus strain for several different τ_{SRH} values, assuming 5×10^{18} cm⁻³ n-type doping. For strains below 1.0%, there is almost no difference between the curves for τ_{SRH} of 10 ns or greater. At 2.0% strain, the 10-ns curve shows a noticeably higher threshold than the 100-ns and 10- μ s curves, and at 3.0% strain even the 100-ns curve has started to diverge from the 1- μ s and 10- μ s curves. The explanation for this phenomenon is that improving τ_{SRH} is only helpful when the net carrier lifetime is limited by the defect-assisted recombination process as opposed to other mechanisms such as Auger recombination. In the high threshold regime, the Auger-limited lifetime is about 1 ns or less, and so it makes little difference whether τ_{SRH} is 1 μ s or 10 ns. In the low-threshold regime, however, the Auger-limited lifetime can be closer to 300 ns. In this case, reducing τ_{SRH} from 1 μ s to 10 ns will dramatically reduce the net carrier lifetime and thus increase the threshold by more than an order of magnitude. The key takeaway of

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4 this result is that while material quality is already important to improving the performance of
5 Ge lasers, it will become even more important as techniques such as band engineering and
6 n-type doping start to lower lasing thresholds.
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9 Another important effect of the defect-limited carrier lifetime is that it also affects the
10 optimal doping level: it is known that too much n-type doping can be harmful [6]. From Fig.
11 3, we indeed observed that increasing the doping too much will cause the threshold to
12 increase. Also, as can be inferred from plots for various τ_{SRH} values in Fig. 3, the optimal
13 amount of n-type doping depends quite strongly on the τ_{SRH} . For instance, looking at the top
14 of each plot in Fig. 3, we see that for the case of 3.0% biaxial tensile strain, the threshold is
15 minimized at a doping of more than $1 \times 10^{19} \text{ cm}^{-3}$ when τ_{SRH} is 100 ps. But for the case of a 1
16 μs lifetime, we observe that the threshold is minimized for an n-type doping of less than
17 $5 \times 10^{18} \text{ cm}^{-3}$. This “optimal doping,” i.e. the doping value which minimizes the threshold, is
18 shown explicitly in Fig. 5(b), wherein we consistently observe that the optimal doping value
19 is lower when τ_{SRH} is higher. On a practical level, this result means that n-type doping will
20 become less useful as researchers develop ways to grow Ge with fewer defects and thus
21 longer τ_{SRH} . As shown in Fig. 5(b), assuming 1.5% biaxial strain which has recently been
22 realized in Ge-on-Si [28], we find for τ_{SRH} of 1 ns that n-type doping will remain useful for
23 concentrations up to $7.2 \times 10^{19} \text{ cm}^{-3}$. However, if improvements in Ge epitaxy can extend
24 τ_{SRH} to 100 ns, n-type doping will only be useful at concentrations up to $3.4 \times 10^{19} \text{ cm}^{-3}$
25 (assuming again 1.5% strain). Such doping levels are significantly lower than what has
26 already been achieved experimentally [29]. Thus, while very heavy n-type doping may
27 improve a Ge laser’s threshold now that τ_{SRH} are quite small [10], as the material quality of
28 Ge improves, it will become necessary to actually reduce the n-type doping from present
29 levels in order to achieve the best possible laser performance.
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32 In summary, we show that it is critically important to improve the defect-limited carrier
33 lifetime in order to achieve a high efficiency LED, indicating that much work is needed on
34 improving material quality [11]. Given that state-of-the-art epitaxial Ge has a defect-limited
35 carrier lifetime of only $\sim 1 \text{ ns}$, our modeling suggests that improving this lifetime to $\sim 100 \text{ ns}$
36 would proportionally improve the efficiency of a Ge LED by two orders of magnitude. This
37 makes lifetime improvements even more critical to LED device performance than band
38 engineering such as biaxial strain. Our modeling also shows that improving the
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defect-limited carrier lifetime is critical for achieving a low-threshold Ge laser. We show that the defect-limited carrier lifetime will become even more important as techniques such as band engineering start to lower lasing thresholds. Interestingly, we observe a negative interaction between material quality and n-type doping: as the material quality improves and reduces the lasing threshold, this will make n-type doping less helpful. This work suggests that to realize a high-efficient Ge LED and a low-threshold Ge laser, we should put more research effort into improving material's quality which has been overlooked so far.

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Figure Captions

Fig. 1. The bandstructure of Ge with 2.0% biaxial tensile strain computed by tight-binding. (a) 2D cross-sectional view. Black dashed horizontal lines are visual aids to help illustrate the Γ -L energy separation under tensile strain. (b) 3D cross-sectional view ($k_z=0$). The x- and y-components of the wavevector ($\mathbf{k}$) are shown, with units given as multiples of the inverse lattice constant ($1/a$).

Fig. 2. Internal quantum efficiency of a Ge double-heterostructure LED for various τ_{SRH} values. Doping is assumed to be $1 \times 10^{19} \text{ cm}^{-3}$. (a) Linear scale in y-axis. (b) Logarithmic scale in y-axis.

Fig. 3. Threshold current density vs. biaxial strain and n-type doping, shown for various τ_{SRH} values. In all cases a double heterostructure design with a 300-nm thick Ge active region and zero optical cavity loss is assumed.

Fig. 4. Emission wavelength vs. biaxial tensile strain and n-type doping. Ge thickness is assumed to be 300 nm with an optical cavity loss of zero and $\tau_{\text{SRH}}=100 \text{ ns}$.

Fig. 5. (a) Threshold current density vs. biaxial strain assuming a 300-nm thick Ge active region with $5 \times 10^{18} \text{ cm}^{-3}$ n-type doping, shown for various τ_{SRH} values. (b) Optimal doping vs. biaxial strain, shown for various τ_{SRH} values. In all cases a double heterostructure design with zero optical cavity loss is assumed.

Figures

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