Anomalous Threshold Reduction from <100> Uniaxial Strain for a Low-Threshold Ge Laser

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Abstract

We theoretically investigate the effect of <100> uniaxial strain on a Ge-on-Si laser. We predict a dramatic ~200x threshold reduction upon applying sufficient uniaxial tensile strain to Ge. This anomalous reduction is explained by how the topmost valence bands split and become anisotropic with uniaxial tensile strain. Approximately 3.2% uniaxial strain is required to achieve this anomalous threshold reduction for $1 \times 10^{19} \text{ cm}^{-3}$ n-type doping, and a complex interaction between strain and n-type doping is observed. Achieving this critical uniaxial strain level for the anomalous threshold reduction is dramatically more relevant to practical devices than realizing a direct band gap.

Keywords

Germanium; Optical Interconnects; Laser; Uniaxial Strain

Strain engineering has been traditionally important in semiconductor device technology because of its ability to substantially modify a material's bandstructure and thereby change its electrical and optical properties in useful ways [1,2]. Tensile strain engineering in germanium (Ge) has been an especially major research topic within the silicon- (Si-) compatible photonics community [3,4]. Ge can be readily integrated on Si and, upon application of sufficient tensile strain, it has the potential to become an efficient gain medium for a CMOS-compatible light source [4–6], with possible applications in both on-chip optical interconnects [7,8] and infrared sensing [9]. Many theoretical analyses of biaxially strained Ge lasers exist in literature [4–6,10], but modeling of uniaxially strained Ge lasers remains much more limited. This is a serious deficiency in light of recent experimental advances in achieving large, spatially homogeneous CMOS-compatible $\langle 100 \rangle$ uniaxial strains in Ge [8,11], including up to 5.7% uniaxial strain which is sufficient to turn Ge into a direct bandgap semiconductor [12].

Here we present extensive theoretical modeling of the threshold current density in $\langle 100 \rangle$ uniaxially strained Ge lasers. One of the most important and surprising features we predict is the sudden reduction of threshold current by more than two orders of magnitude on application of uniaxial tensile strain in the range of 2-4%. The exact amount of critical strain needed for this dramatic reduction depends on the amount of n-type doping in the Ge, and the anomalous threshold reduction itself is due to valence band (VB) splitting. Under uniaxial tensile strain, the topmost VB becomes anisotropic with the heavy-hole mass along the strain axis and the light-hole mass along the other two axes, respectively [2,13–16]. The second VB gains the opposite characteristic. If the splitting of the two topmost VBs is large enough with increasing strain, there can be a sudden change in lasing behavior [4]. This is because both light-hole and heavy-hole bands contribute to the optical gain when the VB splitting is small, but when the splitting is large only the top VB will contribute to the gain [4]. For uniaxial strain, this VB splitting is particularly beneficial because it causes the top VB to have smaller density of states compared to the second VB, thereby dramatically reducing the density of states at the top VB [2,13,14]. This particularity of uniaxial strain has been somewhat overlooked by researchers despite its immense importance. Here we discuss this VB splitting effect of uniaxial strain for reducing Ge laser threshold and show the importance of properly choosing the design

parameters of n-type doping and uniaxial strain in order to realize a truly practical Ge laser with a low threshold.

We can calculate how the band edges of Ge change under $\langle 100 \rangle$ uniaxial strain using deformation potential theory [2] as shown in Fig. 1. We find that it takes 4.6% uniaxial strain to achieve a direct bandgap. The major difference between uniaxial and biaxial strain concerns the VB splitting that occurs under strain. Whereas for $\langle 100 \rangle$ biaxial tensile strain the top VB retains a mostly heavy-hole character with the heavy-hole mass along two strain-parallel axes, under $\langle 100 \rangle$ uniaxial strain the top VB retains a mostly light-hole character with the heavy-hole mass only along one strain-parallel axis [13,14,16]. We will see through laser modeling how this distinction concerning VB splitting will play a very major role in reducing the threshold with uniaxial strain.

Having determined precisely how the band edges change with uniaxial strain, we can now compute the threshold current density as a function of uniaxial strain and n-type doping following the method we employed previously in Ref. 4. For every strain value, we calculate the quasi-Fermi levels as a function of carrier densities assuming Fermi-Dirac carrier statistics and the band edges of Fig. 1. The inset of Fig. 1 shows the amount of VB splitting as a function of uniaxial strain. Then, we compute the net optical gain using the strain-dependent absorption coefficient of Ref. 17 and the empirical free carrier absorption relation of Ref. 1, and determine the steady-state injected carrier density at the threshold condition (i.e. when the net optical gain equals to the assumed resonator loss which is assumed to be zero in this work). Finally, we convert the steady-state injected carrier density to current density by using Ge's recombination coefficients [1]. We assume a 100% injection efficiency using the rate equation which assumes the amount of pumping per unit volume to equal the amount of recombination from all sources, including defect-assisted Shockley-Reed-Hall (SRH) recombination, radiative recombination from the direct transition, radiative recombination from the indirect transition, and both forms of Auger recombination. The defect-assisted SRH recombination lifetime was chosen to be 100 ns. The use of the strain-dependent absorption coefficient of Ref. 17 allows us to properly treat the separate contributions of the two allowed interband transitions, Γ -1st VB and Γ -2nd VB, which are indicated in Fig. 2. In this modeling we presume a double heterostructure design with perfect carrier confinement and a 300nm-thick Ge active region that always

lases at the wavelength of maximum net gain [4,18].

VB splitting, illustrated in Fig. 2, occurs under any non-hydrostatic strain and will prove particularly important for our analysis. Under $\langle 100 \rangle$ uniaxial tensile strain the top VB has light-hole mass along two strain-perpendicular axes, which results in a dramatically reduced density of states at the top of the VB [2,13,16]. The light- and heavy-hole masses were chosen to be $0.043 m_0$ and $0.34 m_0$, respectively, where m_0 is the free electron rest mass [19]. This plays a major role in determining the threshold current density and preferred emission wavelength as a function of uniaxial strain and n-type doping, computed using the previously described method and shown in Fig. 3.

From Fig. 3, we observe that uniaxial strain exponentially reduce the threshold current of a Ge laser and dramatically redshift the preferred emission wavelength. These enhancements with strain continue even after a direct bandgap has been achieved at 4.6% uniaxial strain as we show here in Fig. 3(a) and indicates that there is no special benefit to achieving a direct bandgap with respect to laser performance. More importantly, there are two distinct regimes due to the VB splitting: after about 2-4% uniaxial strain it becomes possible to achieve particularly dramatic reductions in threshold coupled with an abrupt jump in wavelength. This two-regime phenomenon is where uniaxial strain becomes very promising. For uniaxial strain we find that exceeding a certain critical value causes an abrupt and immediate drop in the threshold itself. This phenomenon can be seen more clearly in Fig. 4, which is a 3D surface plot of Fig. 3(a). This sudden drop in threshold under uniaxial strain can exceed two orders of magnitude depending on the doping level.

When the VB splitting becomes sufficiently large to allow lasing using only the Γ -1st VB transition, the threshold will be dramatically smaller due to the much smaller density of states in the 1st VB. In addition, due to the smaller joint density of states for the Γ -1st VB transition, a large amount of VB splitting (and thus a large amount of uniaxial strain) is required before the gain from this Γ -1st VB transition is alone sufficient to overcome free carrier absorption. This is why a comparatively large 2-4% uniaxial strain is required to achieve disproportionate threshold reductions.

As shown in Fig. 5, employing n-type doping (or increasing the n-type doping level) allows this regime change to happen at smaller strain values whereupon the discontinuity is less pronounced. At $1 \times 10^{20} \text{ cm}^{-3}$ n-type doping, the regime change occurs at $\sim 1.1\%$ strain

and there is no discontinuity, just a kink. At $5 \times 10^{19} \text{ cm}^{-3}$ doping, the regime change occurs at $\sim 1.8\%$ strain and there is a discontinuity whereupon the threshold abruptly drops by a factor of ~ 5 x. At $1 \times 10^{19} \text{ cm}^{-3}$ doping, the regime change occurs at $\sim 3.2\%$ strain and there is a discontinuity whereupon the threshold abruptly drops by a factor of ~ 200 x. This makes n-type doping a double-edged sword with respect to improving uniaxially strained Ge lasers. On one hand, applying n-type doping makes the critical strain smaller and thus easier to reach, but on the other hand n-type doping reduces the benefits that can be realized by exceeding this critical strain. This fits with the general theme of moderate n-type doping being useful to strained Ge laser performance, but too much n-type doping proving to be quite harmful [4].

This means that it is truly imperative to reach this critical strain level for uniaxial strain if a low-threshold Ge laser is to be realized. This critical strain represents a hard boundary between a very high threshold regime and a very low threshold regime. For the case of $1 \times 10^{19} \text{ cm}^{-3}$ n-type doping, this critical strain is about 3.2% along the $\langle 100 \rangle$ direction which is considerably smaller than the 4.6% $\langle 100 \rangle$ uniaxial strain needed to achieve a direct bandgap. What this means is that, in order to dramatically reduce the lasing threshold, it is much more important to properly choose design parameters such as n-type doping and uniaxial strain level than to simply pursue the 4.6% uniaxial strain for achieving the direct bandgap Ge which has been the central objective of many researchers.

In summary, we have performed in-depth modeling of $\langle 100 \rangle$ uniaxial strain, with a particular focus on the effect of VB splitting. Through the modeling, we find that with uniaxial strain there exists a discontinuity in the threshold versus strain curve such that the threshold abruptly drops when the strain exceeds a critical value ($2\text{-}4\%$ depending on the n-type doping level). This special feature from uniaxial strain comes from the fact that under uniaxial tensile strain the top VB retains a mostly light-hole character. While our results indicate that there is no practical utility in striving for a direct bandgap at 4.6% uniaxial strain, there is immense utility in exceeding the easier goal of $\sim 4\%$ uniaxial strain which unlocks the anomalous threshold reduction in undoped Ge. With $5 \times 10^{19} \text{ cm}^{-3}$ n-type doping, a doping level which is practical [20], the critical uniaxial strain for which researchers must strive becomes as low as 1.8% . This is considerably lower than what has been reported in stressed micro-bridge structures [8,11,12], and even techniques

incorporating an optical cavity now report strains very close to this value [21]. This indicates that practical realization of a low threshold uniaxially strained Ge laser may be well on the way to fruition if recent advances in strain engineering can be combined with effective device integration.

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Figure Captions

Fig. 1. Ge's direct (Γ) and indirect (L) bandgap energies vs. $\langle 100 \rangle$ uniaxial strain. The inset shows the amount of VB splitting as a function of uniaxial strain.

Fig. 2. Illustration of the distinct Γ -1st VB and Γ -2nd VB transitions which can both contribute to optical gain.

Fig. 3. (a) Threshold current density (color scale) of a double heterostructure Ge laser vs. uniaxial tensile strain and n-type doping. (b) Emission wavelength (color scale) vs. uniaxial tensile strain and n-type doping. Ge thickness is assumed to be 300 nm with an optical cavity loss of zero and a defect-limited minority carrier lifetime of 100 ns. The blank region in the bottom left corner is due to the cutoff of the simulation bounds, i.e. thresholds greater than 1000 kA/cm³.

Fig. 4. Threshold current density vs. uniaxial tensile strain ($\langle 100 \rangle$ orientation) and n-type doping. A double heterostructure design with a 300nm-thick Ge active region and zero optical cavity loss is assumed.

Fig. 5. (a) Threshold current density of a Ge laser vs. uniaxial tensile strain ($\langle 100 \rangle$ orientation) for different doping conditions. (b) Emission wavelength of a Ge laser vs. uniaxial tensile strain ($\langle 100 \rangle$ orientation) for different doping conditions. The outlier data points in the discontinuity region of figure (a) are artifacts from linear interpolations in the vicinity of the discontinuity.

Figures

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