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Abstract: A tensile-strained GeSn/SiGeSn multiple quantum well (MQW) laser wrapped in Si$_3$N$_4$ liner stressor is designed and characterized theoretically. A biaxial tensile strain is introduced into the GeSn/SiGeSn MQW laser by the Si$_3$N$_4$ liner stressor. The boosting effects of tensile strain on the threshold current density $j_t$ and optical gain in GeSn/SiGeSn lasers are attributed to the modulation of energy band structure and carrier distribution in the GeSn wells. Tensile-strained Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.839}$Sn$_{0.144}$ MQW laser wrapped in 500 nm Si$_3$N$_4$ liner stressor achieves a $j_t$ reduction from 476 to 168 A/cm$^2$ and a significant enhancement of optical gain, as compared to the relaxed control device without Si$_3$N$_4$. The design of GeSn/SiGeSn MQW structure wrapped in Si$_3$N$_4$ liner stressor provides a practical way to realize high performance GeSn based mid-infrared laser.

Index Terms: GeSn/SiGeSn, quantum well laser, Si$_3$N$_4$ liner stressor.

1. Introduction

Nowadays, the obstacle to achieve a fully functional silicon photonic platform is the realization of a monolithically integrated laser [1]. As a “fab”-compatible material, germanium (Ge) has been intensely explored as one of the most promising gain media due to its superior optoelectronic properties over silicon [2]–[4]. However, the indirect bandgap property of Ge limits its luminous efficiency. The new group IV alloy, germanium-tin (GeSn), has attracted great attention due to the fact that both theoretical and experimental studies indicate that GeSn becomes a direct bandgap material at a Sn composition of 6.5%, or less than 11% [5]–[8], making it a very promising candidate as the gain medium in lasers [8], [9].
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Fig. 1. 3D schematic of the Ge\textsubscript{1−x}Sn\textsubscript{x}/Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z} MQW laser wrapped in a Si\textsubscript{3}N\textsubscript{4} liner stressor. The coordinate axes and the key parameters of the device are shown.

The optically pumped GeSn lasers have been reported and the lasing performance was expected to be further enhanced via increasing Sn composition and improving the material quality [10]–[13]. However, epitaxial growth of GeSn with high Sn composition is still challenging due to the very limited solid solubility of Sn in Ge. In addition, the thermal stability of GeSn film becomes poorer with higher Sn content, which poses a challenge for device fabrication [14]–[18]. It was reported that inducing a tensile strain into GeSn alloys reduces the Sn composition needed for realization of direct bandgap [6], [8], [19], benefiting their luminescence characteristics [20], [21]. Using Si\textsubscript{3}N\textsubscript{4} as external stressor is an effective and practical technique to induce tensile or compressive strain into semiconductor [22]–[25].

In this paper, we design a GeSn/SiGeSn multiple quantum well (MQW) laser wrapped in Si\textsubscript{3}N\textsubscript{4} liner stressor. The effect of tensile strain induced by the Si\textsubscript{3}N\textsubscript{4} liner stressor on the optical gain and threshold current \( J_{\text{th}} \) in the GeSn/SiGeSn MQW laser is investigated theoretically. The dependence of laser performance on Sn composition, injected carrier density \( n_{\text{injected}} \), and quantum well number \( n_{\text{well}} \) is also discussed.

2. Device Structure of GeSn/SiGeSn MQW Laser Wrapped in Si\textsubscript{3}N\textsubscript{4} Liner Stressor

Fig. 1 depicts the 3D schematic of Si\textsubscript{3}N\textsubscript{4} liner stressor wrapping around Ge\textsubscript{1−x}Sn\textsubscript{x}/Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z} MQW microdisk laser on Ge\textsubscript{1−t}Sn\textsubscript{t} buffer on Ge/Si virtual substrate. If the thickness of GeSn higher than the critical thickness, the film is partially relaxed [10], [11], so Ge\textsubscript{1−t}Sn\textsubscript{t} buffer with higher Sn composition than Ge\textsubscript{1−x}Sn\textsubscript{x} active layer, i.e., \( t > x \) is used to achieve fully relaxed Ge\textsubscript{1−x}Sn\textsubscript{x}/Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z} MQW. The active region of device consists of Ge\textsubscript{1−x}Sn\textsubscript{x} well and Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z} barrier are 7 nm and 10 nm, re-spectively. Material compositions are adjusted to provide lattice-match to Ge\textsubscript{1−t}Sn\textsubscript{t} and type-I heterojunction at \( \Gamma \) point at the interface of fully relaxed Ge\textsubscript{1−x}Sn\textsubscript{x}/Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z}. The lattice constants of Ge\textsubscript{1−x}Sn\textsubscript{x} and Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z} were obtained by linear interpolation between the lattice constants of Si, Ge, and \( \alpha \)-Sn, which are 5.43095 Å, 5.64613 Å, and 6.48920 Å [26]. The bandgap of the materials were calculated using the Vegard’s law, with the consideration of bowing parameters, which were taken from [6], [27], [28]. It should be noted that all the bowing parameters have been modified according to the experimental results. According to [29], as \( x \) is fixed in Ge\textsubscript{1−x}Sn\textsubscript{x}, \( y \) or \( z \) in Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z} are adjusted to achieve lattice-matched heterostructure maximum conduction band offset at type-I Ge\textsubscript{1−x}Sn\textsubscript{x}/Si\textsubscript{1−y−z}Ge\textsubscript{y}Sn\textsubscript{z} interface. The microdisk structure can be formed by selectively removing the Ge\textsubscript{1−x}Sn\textsubscript{x} and Ge layers underneath. Then 500 nm Si\textsubscript{3}N\textsubscript{4} liner stressor with residual compressive strain of \( \sim 2.4 \) GPa is formed by low-temperature plasma enhanced chemical vapor deposition. Top and bottom metal electrodes can be formed through the contact holes in Si\textsubscript{3}N\textsubscript{4}. Simulations demonstrate that the influence of contact holes on strain distribution in device is negligible.
3. Results and Discussion

3.1. Strain Profiles in GeSn Wells

A finite element (FEM) simulation was performed to analyze the strain distribution in the lattice-matched GeSn/SiGeSn MQW laser wrapped in a 500 nm Si$_3$N$_4$ liner stressor with COMSOL Multiphysics software. The elastic stiffness tensor $C_{ij}$ of GeSn and SiGeSn were calculated by a linear interpolation based on $C_{ij}$ of Si, Ge, and $\alpha$-Sn. The $C_{ij}$ of materials used in simulation are listed in Table 1. We assumed that all the surfaces of the device are assumed to move freely, except for the bottom surface. Fig. 2 shows the strain distributions on the normal and radial cross section.

Table 1

<table>
<thead>
<tr>
<th>Material</th>
<th>$C_{11}/C_{22}$ (GPa)</th>
<th>$C_{12}$ (GPa)</th>
<th>$C_{13}/C_{23}$ (GPa)</th>
<th>$C_{22}$ (GPa)</th>
<th>$C_{24}/C_{55}$ (GPa)</th>
<th>$C_{33}$ (GPa)</th>
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</thead>
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<td>Ge</td>
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<td>47.70</td>
<td>47.70</td>
<td>128.70</td>
<td>66.70</td>
<td>66.70</td>
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<tr>
<td>$\alpha$-Sn</td>
<td>69.00</td>
<td>29.30</td>
<td>29.30</td>
<td>69.00</td>
<td>36.20</td>
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<td>Si</td>
<td>165.64</td>
<td>63.94</td>
<td>63.94</td>
<td>165.64</td>
<td>79.51</td>
<td>79.51</td>
</tr>
<tr>
<td>Si$_3$N$_4$</td>
<td>439.17</td>
<td>181.85</td>
<td>149.91</td>
<td>556.98</td>
<td>114.38</td>
<td>135.93</td>
</tr>
</tbody>
</table>
Fig. 3. Energy band diagrams of (a) unstrained and (b) tensile strained Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW laser wrapped in a 500 nm Si$_3$N$_4$ liner stressor. The values of the built-in electric field are 2.6 and 2.1 MV/m in the unstrained and strained devices, respectively. The contour plots for the strain along [100], [010], and [001] directions in the normal cross section plane are denoted by $\varepsilon_{[100]}$, $\varepsilon_{[010]}$, and $\varepsilon_{[001]}$, respectively. It should be noted that X, Y, and Z represent [100], [010], and [001] directions, respectively. It is observed that $\varepsilon_{[100]}$ and $\varepsilon_{[010]}$ are tensile, and $\varepsilon_{[001]}$ is compressive. At the center of the GeSn layer of GeSn/SiGeSn MQW laser, the values of $\varepsilon_{[100]}$, $\varepsilon_{[010]}$, and $\varepsilon_{[001]}$ are 0.85%, 0.85%, and $-0.77\%$, respectively. It should be noted that the fringe region of the microdisk has the smaller magnitude of strain compared to the central region, which leads to larger bandgap of Ge$_{1-x}$Sn$_x$ quantum wells in fringe regions, widening the emission spectrum of the laser. Simulation results indicate that the impact of $x$ on strain distribution in device was negligible, with the Sn composition ranging from 0 to 0.1. It is noted that GeSn/SiGeSn QW structures are lattice matched to the GeSn buffer for all the material compositions, and the strain is only introduced by the Si$_3$N$_4$ liner stressor.

3.2. Energy Band Structure and Carrier Distribution in GeSn/SiGeSn MQW

The energy band diagrams and carrier distribution in the MQW structures were computed utilizing multi-band k-p method. The deformation potentials for the conduction and valence bands and the Luttinger parameters for GeSn and SiGeSn alloys were taken from [29]. The calculated strains at the central region of GeSn/SiGeSn disk in the device were converted into the strain tensor as the input variables of the k-p Hamiltonian. Fig. 3(a) and (b) illustrate the band diagrams of the relaxed Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW laser and the strained device wrapped in a 500 nm Si$_3$N$_4$ liner stressor, respectively. The ground sub-band energy levels at L and $\Gamma$ conduction valleys, and heavy-hole (HH) and light-hole (LH) bands in Ge$_{0.90}$Sn$_{0.10}$ quantum wells, and the corresponding wave functions are also presented. It can be found that electron and hole are both confined in Ge$_{0.90}$Sn$_{0.10}$ wells, which is in favor of the optical recombination of carriers. The tensile strain induced bandgap reduction in GeSn is attributed to the lowering of conduction valleys in energy and the non-degeneracy of HH and LH bands. It should be noted that the $\Gamma$ conduction valley has a more rapid decline in energy in comparison with L valley thanks to the larger deformation potential. The distribution of electrons in $\Gamma$ and L conduction valleys in GeSn wells are extracted and depicted in Fig. 4, which has a great impact on the $J_n$ and the optical gain of the devices. The increase of electron occupation probability in $\Gamma$ conduction valley is conducive to the improvement of optical emission performance in lasers. The electron concentrations in $\Gamma$ and L valleys are...
Fig. 4. $n_{e,Γ}/n_{e,\text{total}}$ for (a) unstrained and (b) tensile strained GeSn/SiGeSn MQW lasers with a 500 nm Si$_3$N$_4$ liner stressor. The Sn compositions of GeSn wells in devices vary from 0 to 10% in steps of 2%. The performance of the device is affected by the temperature, which has an impact on $n_{e,Γ}/n_{e,\text{total}}$. As $n_{e,Γ}/n_{e,\text{total}}$ is less than $10^{19}$ cm$^{-3}$, $n_{e,Γ}/n_{e,\text{total}}$ in GeSn wells demonstrates a substantial improvement with the increasing of Sn composition, where the total electron concentration $n_{e,\text{total}}$ is the sum of those in $Γ$ and $L$ valleys ($n_{e,Γ} + n_{e,L}$). With a fixed Sn composition, the tensile strained GeSn well exhibits a several times higher $n_{e,Γ}/n_{e,\text{total}}$ in comparison with the relaxed one, due to the more pronounced decreasing in energy of energy states in $Γ$ conduction valley compared to the $L$ valley under the tensile strain.

3.3. Threshold Current and Gain Coefficient in the Laser

Fig. 5 shows the relationship between the $ΔE_Γ$ and the $n_{\text{injected}}$ in relaxed and tensile strained GeSn/SiGeSn MQW lasers with different Sn compositions. The triangular symbols indicate the values of $n_{\text{injected}}$ for the onset of population inversion, denoted by $n_{\text{onset,pi}}$, in the devices with different Sn compositions. As the Sn composition increases, the $n_{\text{onset,pi}}$ decreases. Under the tensile strain, the $n_{\text{onset,pi}}$ is further reduced due to the decrease of the sub-bandgap $E_{\text{sub}}$ in GeSn wells. The tensile strained Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW laser demonstrates a $n_{\text{onset,pi}}$ of $5 \times 10^{18}$ cm$^{-3}$, which is much lower than that of the relaxed device, $3.8 \times 10^{18}$ cm$^{-3}$.

The effects of tensile strain, $n_{\text{injected}}$, and Sn composition on the $g$ of the GeSn/SiGeSn MQW laser are analyzed, where the optical gain coefficient $g$ consists of two parts $g_{Γ-LH}$ and $g_{Γ-HH}$, which are the gain coefficients between the $Γ$ valley of conduction band and the LH and HH, respectively. Fig. 6(a) and (b) depict the impacts of $n_{\text{injected}}$ on $g_{Γ-LH}$ and $g_{Γ-HH}$, respectively, for the Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.134}$ and Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW lasers. The results show that both $g_{Γ-LH}$ and $g_{Γ-HH}$ of devices are improved with the increase of Sn component. The $g_{Γ-LH}$ of strained lasers is significantly enhanced compared with the relaxed devices, which is
due to the modulation effect of tensile strain on the energy band structures in GeSn. As shown in Fig. 6(b), the $g_{\Gamma - HH}$ of strained GeSn/SiGeSn lasers is lower in comparison with the relaxed devices, which is caused by the reduction of the effective mass of the HH under tensile strain. In relaxed GeSn/SiGeSn MQW lasers, the $n_{\text{injected}}$ at the $g_{\Gamma - LH}$ of zero is less than that at $g_{\Gamma - HH} = 0$. This is attributed to the fact that the ground state of LH is lower in energy compared to that of HH in GeSn quantum wells due to the quantum confinement effect [Fig. 3(a)]. For tensile-strained devices, it is the reverse, which is due to the splitting of HH and LH.

As the threshold characteristics are calculated, the free carrier absorption and mirror loss of the devices are considered. Carrier absorption loss $\alpha_f$ is calculated by $\alpha_f(\lambda) = AN\lambda^a + BP\lambda^b$, where $A$, $B$, $a$, and $b$ are constants, and $N$ and $P$ are electron and hole densities, respectively [33]. The values of $A$, $B$, $a$, and $b$ of Ge taken from [33] are utilized. The mirror loss is assumed to be 50 cm$^{-1}$ [33]. Fig. 7 depicts the dependence of $n_{th}$ and $J_{th}$ on the Sn composition for the relaxed and strained lasers. Here, $n_{th}$ is the threshold value of $n_{\text{injected}}$ for laser and $L_z$ is the thickness of the potential well. It is clarified that the effects of defects and surface roughness induced by the incorporation of Sn atoms on $g$ and $J_{th}$ were not taken into account. With the development of growth technique for GeSn, the crystalline quality of GeSn alloys has been significantly improved. Surface RMS roughness less than 2 nm can be achieved for the partially relaxed GeSn grown on Si [34]. GeSn photodiodes with very low dark current and high responsivity and GeSn channel transistors
with high carrier mobility were demonstrated [35]–[41]. Compared to the relaxed device, the $n_{th}$ and $J_{th}$ in the tensile strained Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW laser decreases from $4.69 \times 10^{18}$ to $0.75 \times 10^{18}$ cm$^{-3}$, and from 476 to 168 A/cm$^2$, respectively. It should be noted that the tensile strain not only affects the optical gain and $\lambda$. Assuming the laser $\lambda$ is directly determined by the $E_{\text{sub}} - G$, the $\lambda$ of relaxed and tensile strained Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW lasers are about 2.3 and 3.1 $\mu$m, respectively. The emission intensity of the MQW laser is proportional to the product of the optical confinement factor $\Gamma$ and optical gain. For the transverse electric field wave (TE) and transverse magnetic field wave (TM), optical confinement factors, denoted by $\Gamma^\text{TE}_{\text{MQW}}$ and $\Gamma^\text{TM}_{\text{MQW}}$, respectively, can be calculated by [42], [43].

Fig. 8(a) shows the confinement factors $\Gamma^\text{TE}_{\text{MQW}}$ and $\Gamma^\text{TM}_{\text{MQW}}$ in the lasers with different $n_{\text{well}}$. The confinement factors of the laser increases with the increase of $n_{\text{well}}$. It should be clarified that the effect of Si$_3$N$_4$ stressor with a refractive index of 2.0 [44] on the confinement factors are not considered. Compared with the relaxed device, the tensile strained GeSn/SiGeSn lasers exhibits the lower confinement factors due to the redshift of operation $\lambda$. Fig. 8(b) depicts the optical gain $\alpha$ as a function of injected current density $J$ for the relaxed and tensile strained MQW
lasers. To achieve the same $\alpha \ (1 - 200 \text{ cm}^{-1})$, tensile strained Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW laser has the significantly reduced $J$ compared to the relaxed Ge$_{0.90}$Sn$_{0.10}$ device. Furthermore, at the same operation $\lambda$ of 2.3 $\mu$m, strained Ge$_{0.96}$Sn$_{0.04}$/Si$_{0.272}$Ge$_{0.611}$Sn$_{0.115}$ device exhibits the improved $J$ in comparison with the relaxed Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ laser. The values of $\Gamma_{\text{MQW,TE}} \cdot g_{r-HH}$ and $\Gamma_{\text{MQW,TM}} \cdot g_{r-LH}$ are calculated for the relaxed and tensile strained Ge$_{0.90}$Sn$_{0.10}$/Si$_{0.161}$Ge$_{0.695}$Sn$_{0.144}$ MQW lasers, as shown in Fig. 8(b). It is observed that, in spite of the lower $\Gamma$, the tensile strained laser wrapped in Si$_3$N$_4$ stressor achieves improved $\alpha$ for both TE and TM modes due to the significantly boosted optical gain.

To interpret the effect of the gain medium of the device performance, we define the subband energy difference as $\Delta E = E_L - E_R$. The effective mass of L-bandedge is large, resulting in the large density of states. Due to the fact that injected carriers are filled from lower energy side, carrier leakage to L-band is large for large $\Delta E$. It is concluded that the small value of $\Delta E$ is preferable to increase the material gain. As the tensile strain is applied to the device, the band structure is changed. During the injection of carriers, the increase of electron occupation probability in $\Gamma$ conduction valley lead to the occurrence of population inversion between the $E_{\text{sub}}$ in GeSn wells, which is conducive to the improvement of optical emission performance in lasers.

4. Conclusion

Tensile strained GeSn/SiGeSn MQW laser wrapped in Si$_3$N$_4$ liner stressor is investigated by the analytical calculations. Compared to the relaxed device, both $J_{\text{th}}$ and $g$ can be improved by inducing the tensile strain through Si$_3$N$_4$ stressor. The positive effects of increasing the Sn composition and carrier injection density in the GeSn wells on the devices performance are also demonstrated. Although the $\Gamma$ decreases due to the redshift of emission $\lambda$, the tensile strained GeSn/SiGeSn MQW laser wrapped in Si$_3$N$_4$ liner stressor achieves enhanced $\alpha$ for both TE and TM modes, as compared to the relaxed device.

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