Theoretical Analysis of Strain Effect on Optical Gain in $Ge_{1-x}Sn_x$ Alloys

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***Abstract*—We present a theoretical analysis of strain effect on optical gain in biaxially-stressed $Ge_{1-x}Sn_x$ alloys. The electronic band structure for biaxially-stressed $Ge_{1-x}Sn_x$ alloys is calculated using deformation potential theory and k·p method. For unstrained $Ge_{1-x}Sn_x$ alloys, a Sn content of 6.7% is required to achieve a direct bandgap for providing optical gain. The introduction of tensile strain can further soften the requirements for indirect-to-direct bandgap transition, thereby enhancing optical gain. On the other hand, compressive strain significantly increases the energy difference between the Γ- and L-valley conduction band edges, and hence quenching optical gain in $Ge_{1-x}Sn_x$ alloys.**

I. Introduction

$Ge_{1-x}Sn_x$ alloys have recently been considered a potential material for efficient Si-based lasers [1], [2]. Although pure Ge is an indirect bandgap material, its direct conduction band edge lies just 136.5 meV above the lowest L-valley conduction band edge. This smaller energy difference can be effectively reduced by introducing Sn, another group-IV element. Recent experiments real that indirect-to-direct bandgap transition can occur with a Sn content as small as 6.7% [3]. Enhanced photoluminescence and electroluminescence from $Ge_{1-x}Sn_x$ alloys have been recently reported [3]–[5], as well as first lasing action at low temperatures by optically pumping a GeSn waveguide cavity [6]. However, epitaxial growth of $Ge_{1-x}Sn_x$ films on Si or Ge (buffer) usually induces a considerable residual strain, which could significantly impact the band structure, and hence the optical gain. Therefore an investigation of strain effect on optical gain is necessary in order to reduce the threshold of GeSn lasers.

In this paper, we present a theoretical analysis of strain effect on optical gain of $Ge_{1-x}Sn_x$ alloys. We calculate the strained electronic band structure for biaxially stressed GeSn alloys to predict the required Sn content to achieve indirect-to-direct bandgap transition under different strain conditions. Optical gain spectra of $Ge_{1-x}Sn_x$ alloys under different strain conditions are calculated and compared to show the strain effect.

II. Theoretical Models

The strained band structure of $Ge_{1-x}Sn_x$ alloys is calculated using multi-band k·p method, where the strain effect is considered using deformation potential theory [2]. The parameters for $Ge_{1-x}Sn_x$ used in this calculation are taken from Ref. [2]. The bandgap energy of bulk $Ge_{1-x}Sn_x$ is given by

$$E_{\mathrm{g}}^{\eta}(\mathrm{Ge}_{1-x}\mathrm{Sn}_x) = (1-x)E_{\mathrm{g}}^{\eta}(\mathrm{Ge}) + xE_{\mathrm{g}}^{\eta}(\mathrm{Sn}) - b^{\eta}x(1-x), \quad (1)$$

where $E_{\mathrm{g}}^{\eta}(\mathrm{Ge})$ and $E_{\mathrm{g}}^{\eta}(\mathrm{Sn})$ denote the bulk bandgap energies of Ge and α-Sn, respectively, b^{η} is the bowing parameter, and η denotes different valleys. The bandgap parameters are listed in Table I. After the strained electronic band structures are obtained, the optical gain spectra are calculated using the theoretical model described in Ref. [7].

III. Results and discussions

Fig. 1(a)-(c) shows schematic band structures for tensile-strained, unstrained, and compressive-strained $Ge_{1-x}Sn_x$. For unstrained $Ge_{1-x}Sn_x$, the energy difference between the Γ-valley and L-valley conduction band edges ($\Delta E_{\Gamma L} = E_{\Gamma} - E_L$ with E_{Γ} (E_L) being the Γ-conduction (L-conduction) band edge) can be reduced by the incorporation of Sn. For tensile-strained $Ge_{1-x}Sn_x$, the tensile strain lowers both the Γ-valley and L-valley conduction band edges. However, the Γ-conduction band edge shifts faster than the L-one. As a result, $\Delta E_{\Gamma L}$ can be further reduced to help achieve a direct bandgap. On the other hand, compressive strain lifts the Γ-conduction band with a higher rate than that of L-conduction band, thereby increasing $\Delta E_{\Gamma L}$. Figure 1(d) shows the calculated $\Delta E_{\Gamma L}$ as a function of Sn composition and in-plane strain ε for biaxially-stressed $Ge_{1-x}Sn_x$. Clearly, increasing Sn content and tensile strain can reduce $\Delta E_{\Gamma L}$ and thus transfer the material from fundamentally indirect to direct. On the other hand, compressive strain can increase $\Delta E_{\Gamma L}$ to prevent the material from being direct bandgap materials, so it is an unwanted effect for $Ge_{1-x}Sn_x$ layer gain media. For example, pseudomorphic $Ge_{1-x}Sn_x$ on Ge (VS) cannot be transferred into a direct bandgap material for a epitaxially available Sn content of $x \leq 0.1$

TABLE I
Bandgap energy parameters for bulk $Ge_{1-x}Sn_x$

	E_g(Ge) (eV)	E_g(Sn) (eV)	b (eV)
Γ-valley	0.7985	-0.413	2.42
L-valley	0.664	0.092	0.89

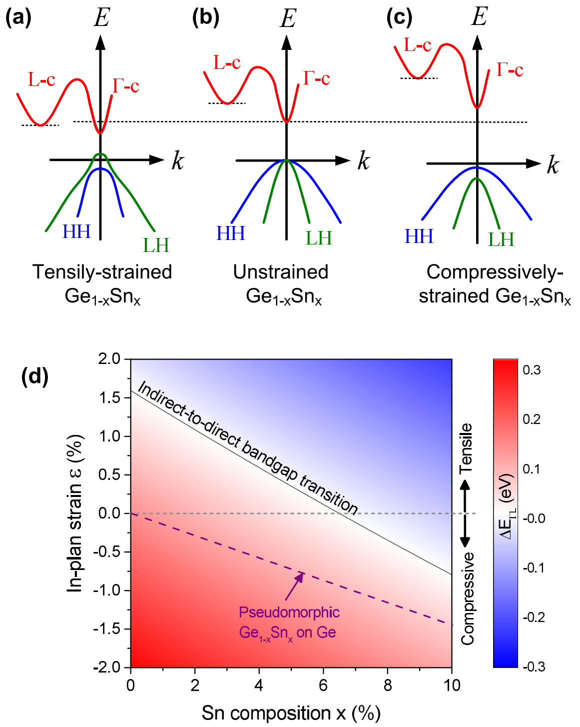

Fig. 1. Comparison of band structures for $Ge_{1-x}Sn_x$ under (a) unstrained condition, (b) tensile-strained condition, and (c) compressive-strained condition.(d) Calculated energy difference between the Γ-valley and L-valley conduction band edges as a function of Sn content and in-plane strain for $Ge_{1-x}Sn_x$.The solid line denotes the indirect-to-direct bandgap transition ($\Delta E_{\Gamma L} = 0$) and the purple dashed line represents pseudomorphic $Ge_{1-x}Sn_x$ on Ge.

Fig. 2 shows the calculated optical gain spectra for biaxially-stressed GeSn alloys at different levels of in-plane strain under an injected carrier density of $n = 1 \times 10^{19}$ cm^{-3}. For unstrained $Ge_{0.95}Sn_{0.05}$, which is an indirect bandgap material, optical gain is not obtainable under this injected carrier density, as shown in Fig. 2(a). However, tensily straining the material can help transfer the material into a direct bandgap material, thereby achieve optical gain. For unstrained $Ge_{0.9}Sn_{0.1}$, which is a direct bandgap material, a peak optical gain of 2194 cm^{-1} is achievable at a photon energy of 494 meV, as shown in Fig. 2(b) If tensile strain is introduced, optical gain can be further enhanced, and the gain spectrum shifts to lower photon energies due to the reduced direct bandgap energy. On the other hand, the introduce of compressive strain weakens, or even quenches, the optical gain because of the increased $\Delta E_{\Gamma L}$. These results indicate that tensile strain is favorable for $Ge_{1-x}Sn_x$ gain media.

In conclusion, we have studied the strain effect on optical gain in $Ge_{1-x}Sn_x$ alloys. It is found that tensile strain can soften the requirements for indirect-to-direct bandgap transition and effectively enhance optical gain. However, compressive strain would weaken the optical gain, thus preventing the material from being used for laser gain media. These results are useful to understand the optical gain behavior for designing efficient GeSn lasers on silicon.

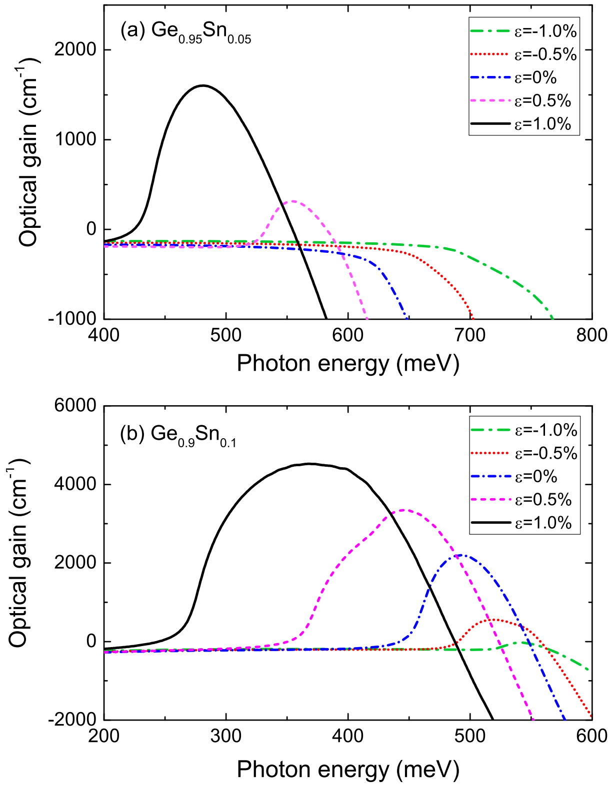

Fig. 2. Calculated optical gain spectra for (a) $Ge_{0.95}Sn_{0.05}$ and (b) $Ge_{0.9}Sn_{0.1}$ alloys under different in-plane strains. The injected carrier density is set to $n = 1 \times 10^{19}$ cm^{-3}

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