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The Theoretical Optical Gain of $\text{Ge}_{1-x}\text{Sn}_x$ Nanowires

Wen Xiong, Wei-Jun Fan,* Zhi-Gang Song, and Chuan-Seng Tan

The electronic structures of $\text{Ge}_{1-x}\text{Sn}_x$ nanowires at the direct Γ -valley and indirect L -valley is calculated using $k \cdot p$ effective-mass theory, and the results demonstrate that $\text{Ge}_{1-x}\text{Sn}_x$ nanowires with large diameter and Sn content can easily be engineered to be the direct-band-gap semiconductor. Furthermore, the optical gain of $\text{Ge}_{1-x}\text{Sn}_x$ nanowires as functions of the injected electron concentration and diameter are obtained. Compared with pure Ge nanowires, a remarkable peak gain can appear in $\text{Ge}_{1-x}\text{Sn}_x$ nanowires even though the injected electron concentration decreases. This is because incorporating Sn into Ge can reduce even reverse the energy difference of minimum bandgap between the direct Γ -valley and indirect L -valley. Therefore, considering the free-carrier absorption loss, one can achieve a positive net peak gain in $\text{Ge}_{1-x}\text{Sn}_x$ nanowires, which indicates that $\text{Ge}_{1-x}\text{Sn}_x$ nanowires can be used as an ideal laser diode candidate in the field of Si-photonics.

The indirect-band-gap nature of semiconductors Si and Ge make their applications harmful in the field of lasers and light emitting diodes (LEDs), although they have been reported for realizing optoelectronic devices.^[1] However, compared with Si, the studies on Ge are more interesting due to the small energy difference in minimum bandgap, namely about 136 meV, between the indirect L -valley and direct Γ -valley in Ge material.^[2] Therefore, a lot of research efforts, including applying the tensile strain^[3] and doping other elements^[4] in Ge material, were devoted to eliminate such small energy difference and obtain the direct band gap. As we know, incorporating tin (α -Sn) into Ge material has been proved to be an effective method to engineer the bandgap of the indirect L -valley and direct Γ -valley,^[5–8] and similar to direct-band-gap III–V or II–VI group semiconductor compounds, GeSn alloys can be integrated into photonic circuits and used as light emitter, which consists of only group IV elements. Recently, apart from the bulk GeSn alloys, many experimental researchers also focused on low-dimensional GeSn-related systems, such as GeSn quantum dots (QDs),^[9,10] nanowires (NWs) or core-shell nanowires,^[11–15] and quantum wells (QWs).^[16,17]

In these experiments, GeSn or strained GeSn related low-dimensional structures with Sn fraction larger than 10% have been realized, and especially GeSn NWs with very high Sn content, namely 22%^[14] and 30%,^[15] have also been reported. Meanwhile, the direct-band-gap GeSn/SiGeSn or GeSn/Si were proved to be the promising systems as QDs or QWs light emitters experimentally. The development of experiments have prompted people to theoretically study the electronic structures and optical properties of GeSn low-dimensional structures. A theoretical model considering the carrier occupations in both the direct Γ -valley and indirect L -valley of GeSn/SiGeSn and Ge/SiGeSn QWs have been developed, and the electronic structures and optical gain of

GeSn/SiGeSn and Ge/SiGeSn QWs as the content of Sn have been investigated.^[18,19] Meanwhile, the theoretical studies about Ge/GeSn and GeSn/SiGeSn QDs have also been performed.^[20,21] However, very little work has been done to systematically investigate the electrical and optical properties of GeSn NWs in theory, although it is important and urgent to understand the influence of Sn content on the electronic structures of GeSn NWs.

In this article, we calculate the electronic structures and optical gain of $\text{Ge}_{1-x}\text{Sn}_x$ NWs by using the effective-mass theory. The electron and hole states of the direct Γ -valley are obtained in the framework of the eight-band $k \cdot p$ theory, whereas for the indirect L -valley, the electron states can also be dealt with via the single-band effective-mass model.^[22] We demonstrate the variation of the optical gain spectra of $\text{Ge}_{1-x}\text{Sn}_x$ NWs with the diameter, Sn content, and injected electron concentration. Furthermore, the net peak gain is also discussed after considering the free-carrier absorption (FCA) loss of $\text{Ge}_{1-x}\text{Sn}_x$ NWs.

At the direct Γ -valley of $\text{Ge}_{1-x}\text{Sn}_x$ NWs, we begin from choosing the eight Bloch basis: $|S\rangle \uparrow, \frac{1}{\sqrt{2}}(|X\rangle + i|Y\rangle) \uparrow, |Z\rangle \uparrow, \frac{1}{\sqrt{2}}(|X\rangle - i|Y\rangle) \uparrow$ and $|S\rangle \downarrow, \frac{1}{\sqrt{2}}(|X\rangle + i|Y\rangle) \downarrow, |Z\rangle \downarrow, \frac{1}{\sqrt{2}}(|X\rangle - i|Y\rangle) \downarrow$, then the eight-band effective-mass $k \cdot p$ Hamiltonian can be written as^[22]

$$H_{\text{eight}} = \begin{pmatrix} H_{\text{int}}^U & 0 \\ 0 & H_{\text{int}}^L \end{pmatrix} + H_{\text{so}} \quad (1)$$

where $H_{\text{int}}^U = H_{\text{int}}^L$ is a 4×4 matrix, and H_{so} is the spin-orbit coupling (SOC) Hamiltonian. It should be noted that the effective-mass parameters L_p , M and N in H_{int}^U (H_{int}^L) can be related to three Luttinger parameters γ_1 , γ_2 , and γ_3 using the following expressions: $L_p = \gamma_1 + 4\gamma_2$, $M = \gamma_1 - 2\gamma_2$, and $N = 6\gamma_3$. The Kane

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energy E_p of $\text{Ge}_{1-x}\text{Sn}_x$ alloy can be set as follows to eliminate the spurious solutions^[22,23]

$$E_p = \frac{3m_0}{m_c} \frac{1}{2/E_g^\Gamma + 1/(E_g^\Gamma + \Delta_{so})} \quad (2)$$

where E_g^Γ and Δ_{so} are the bandgap and spin-orbit splitting energy of $\text{Ge}_{1-x}\text{Sn}_x$ alloy, respectively at the Γ -valley. It should be noted that the above setting about Kane energy E_p will underestimate the quantum confinement effect of the electron states at the Γ -valley, which is important to affect the indirect-to-direct bandgap transition in $\text{Ge}_{1-x}\text{Sn}_x$ NWs. Therefore, in the following numerical calculations and discussions, we will focus on the diameter of $\text{Ge}_{1-x}\text{Sn}_x$ NWs in the range of 12–24 nm, and the quantum confinement effect of $\text{Ge}_{1-x}\text{Sn}_x$ NWs is weak in this range. At the indirect L -valley, the Hamiltonian is as follows^[19]

$$H_L = \frac{\hbar^2}{2m_1^*} (k_z - \pi/a)^2 + \frac{\sqrt{2}\hbar^2}{3m_2^*} k_1 (k_z - \pi/a) + \frac{\hbar^2}{2m_3^*} k_1^2 + \frac{\hbar^2}{2m_4^*} k_2^2 + V_L(r, \theta) \quad (3)$$

where the meanings of the parameters or physical quantities a , m_1^* , m_2^* , m_3^* , m_4^* , k_1 , k_2 , k_z , $V_L(r, \theta)$ and the exact solution of the electron states at the L -valley have been presented in ref. [22]. In the process of diagonalizing Hamiltonian H_L numerically, we must ensure the convergence of the energy of each electron state at the L -valley. Most used parameters, including the effective-mass and the spin-orbit splitting energy, of $\text{Ge}_{1-x}\text{Sn}_x$ alloy in the calculation are taken from ref. [24]. However, the crossover point of bulk $\text{Ge}_{1-x}\text{Sn}_x$ alloy between the direct bandgap E_g^Γ and the indirect bandgap E_g^L is about $x = 11\%$ in ref. [24], which is higher than most recent experimental and theoretical results 6–10%. Therefore, we use the following well-known formula to obtain E_g^Γ and E_g^L

$$E_g^\sigma(\text{Ge}_{1-x}\text{Sn}_x) = (1-x)E_g^\sigma(\text{Ge}) + xE_g^\sigma(\text{Sn}) - b^\sigma x(1-x) \quad (4)$$

where $E_g(\text{Ge}_{1-x}\text{Sn}_x)$, $E_g(\text{Ge})$, and $E_g(\text{Sn})$ represent the bandgap of $\text{Ge}_{1-x}\text{Sn}_x$, Ge and Sn, respectively, and $\sigma = \Gamma$ or L . $E_g^\sigma(\text{Ge})$ and $E_g^\sigma(\text{Sn})$ at the temperature $T = 300$ K are taken from ref. [19]. b is the bowing parameter of $\text{Ge}_{1-x}\text{Sn}_x$ alloy. Chen et al. determined the direct-band-gap parameter $b^\Gamma = 2.1 \pm 0.1$ eV directly in the experiment,^[25] and Polak et al. determined the value $b^\Gamma = 2.43 \pm 0.06$ eV by using state-of-the-art density functional theory methods.^[26] In addition, in refs. [27–29], b^Γ was supposed to 1.8, 1.9, and 1.8 ± 0.2 eV, respectively. For indirect-band-gap parameter b^L , the fitted value was 0.89 eV,^[30] which was adopted by other experimental studies.^[25,31] Meanwhile, b^L in three theoretical studies were found to be 0.64 ± 0.04 ,^[26] 0.90, and 0.91 eV,^[32,33] respectively. Therefore, according to the aforementioned theoretical and experimental studies, b^Γ and b^L are used as 1.90 and 0.90 eV, respectively in our calculation. After using the aforementioned parameters, the crossover point of E_g^Γ and E_g^L is about 8.6%, which matches well with the aforementioned range, namely, 6–10%.

Figure 1a shows the valence band structure of $\text{Ge}_{1-x}\text{Sn}_x$ NWs at the Γ -valley with the diameter $D = 12$ nm and Sn content

$x = 0.08$. Obviously, each hole state is double degenerate and will exhibit strong nonparabolic behavior.^[22] The conduction band structures at the Γ -valley and L -valley are shown in Figure 1b, c respectively with the same diameter and Sn content. We must notice that the energy wave vector dispersion relationship of each electron state in Figure 1c is relative to the minimum L -valley, namely, π/a . Let us focus on the electron states at the L -valley in Figure 1c. Similar to the condition in pure Ge NWs,^[22] each electron state is almost parabolic, which is unlike the case of Γ -valley in Figure 1b. As seen in Equation (3), although the term $k_1(k_z - \pi/a)$ will couple the different order Bessel functions in the envelope wave function of L -valley, the coupling is very weak in $\text{Ge}_{1-x}\text{Sn}_x$ NWs. Therefore, the parabolicity of each electron state at the L -valley is maintained. In addition, as discussed earlier, the energy difference between E_g^Γ and E_g^L can be engineered effectively by incorporating Sn into Ge, which is important to improve the light-emitting efficiency of $\text{Ge}_{1-x}\text{Sn}_x$ alloy. When Sn content $x = 0.08$, the calculated ΔE_g^{bulk} of bulk $\text{Ge}_{1-x}\text{Sn}_x$ alloy, which is defined as $E_g^\Gamma - E_g^L$, is about 9.7 meV. However, for $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $D = 12$ nm and $x = 0.08$, the energies of the ground electron state at the minimum Γ -valley and L -valley are about 0.654 and 0.599 eV, which can be seen from Figure 1b,c. Thus, the direct-band-gap semiconductor is more difficult to be realized in low-dimensional $\text{Ge}_{1-x}\text{Sn}_x$ NWs. One of the main reasons is that the electron effective-mass of $\text{Ge}_{1-x}\text{Sn}_x$ alloy at the Γ -valley is less than that at the L -valley, which will lead to the quantum confinement induced energy of the electron at the Γ -valley larger than that at the L -valley. Figure 1d–f are the same as the corresponding Figure 1a–c, respectively but for the diameter $D = 12$ nm and Sn content $x = 0.11$. Comparing Figure 1d with Figure 1a, we find that not only the shape of the valence band structure but also the energy of each hole state change slightly when x increases from 0.08 to 0.11. As shown in Figure 1e,f, $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $x = 0.11$ is still indirect-band-gap semiconductor, and the energy difference between the ground electron state at the minimum Γ -valley and L -valley is only about 6.10 meV, which indicates that $\text{Ge}_{1-x}\text{Sn}_x$ NWs almost become direct-band-gap semiconductor in this case.

To understand the indirect-to-direct bandgap transition in $\text{Ge}_{1-x}\text{Sn}_x$ NWs, the change of a physical quantity $\Delta E_e^{\Gamma,L}$ with Sn content x and the diameter D is plotted in **Figure 2**, where $\Delta E_e^{\Gamma,L}$ is the energy difference between the lowest electron state at the minimum Γ -valley and L -valley. If $\Delta E_e^{\Gamma,L}$ is less than 0, $\text{Ge}_{1-x}\text{Sn}_x$ NWs becomes the direct-band-gap semiconductor. Clearly, keeping the diameter D fixed, $\Delta E_e^{\Gamma,L}$ will decrease monotonously as the increase in x . When x increases to 0.14, $\text{Ge}_{1-x}\text{Sn}_x$ NWs is direct-band-gap semiconductor whether D is 12 or 24 nm. In addition, as shown in the figure, we can see that direct-band-gap $\text{Ge}_{1-x}\text{Sn}_x$ NWs can be easily obtained with larger diameter D and Sn content x . The same results can also be obtained from **Figure 3**. In Figure 3a, we present the ratio $\Delta n_f/\Delta n$ as functions of D and Δn with $x = 0.05$ when the doping concentration is zero, where Δn is the total injected electron concentration, and Δn_f is the occupied electron concentration at the Γ -valley. As shown in Figure 2, $\text{Ge}_{1-x}\text{Sn}_x$ NWs is indirect-band-gap semiconductor with $x = 0.05$ when $D = 12, 18$ and 24 nm, thus the electron will fill the indirect L -valley first, which is the same as the case of pure Ge NWs.^[22] However, it is worth noting that $\Delta E_e^{\Gamma,L}$ of $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $x = 0.05$ is less than

Figure 1. a) The ten highest hole states and b) eight lowest electron states of $\text{Ge}_{1-x}\text{Sn}_x$ NWs at the Γ -valley with the diameter $D = 12$ nm and Sn content $x = 0.08$, respectively; c) the eight lowest electron states of $\text{Ge}_{1-x}\text{Sn}_x$ NWs at the L -valley with $D = 12$ nm and $x = 0.08$. d–f) The same as (a–c), respectively, but for $x = 0.11$.

Figure 2. The energy difference $\Delta E_e^{\Gamma,L}$ between the lowest electron state at the minimum Γ -valley and L -valley as functions of Sn content x and the diameter D .

that of pure Ge NWs, which can cause the larger ratio $\Delta n_I/\Delta n$ of $\text{Ge}_{1-x}\text{Sn}_x$ NWs when the injected electron concentration Δn is the same. Obviously, it can be seen that the occupied proportion

$\Delta n_I/\Delta n$ will increase with the increment of Δn , and the ratio can be larger than 1% with $D = 12$ nm when Δn increases to $6N_0$. For $\text{Ge}_{1-x}\text{Sn}_x$ NWs with larger diameters, namely, $D = 18$ and 24 nm, the ratio is all below 1% even though $\Delta n = 6N_0$. Figure 3b is the same as Figure 3a but for $x = 0.08$. We can find that the ratios are all larger than 1% when the injected electron concentration decreases from 2–6 N_0 in Figure 3a to $N_0 \approx 3 N_0$ in Figure 3b. In fact, recalling Figure 2, it can be easily found that $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $x = 0.08$ is still indirect-band-gap semiconductor irrespective of the diameters. However, $\Delta E_e^{\Gamma,L}$ will decrease a lot compared with the case of $x = 0.05$ in Figure 3a, which will enhance the occupied proportion $\Delta n_I/\Delta n$ in Figure 3b. When x increases to 0.11 and 0.14, $\Delta n_I/\Delta n$ as a function of Δn are demonstrated in Figure 3c,d, respectively. Note that $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $x = 0.11$ undergoes the transition from indirect bandgap to direct bandgap as the increase in the diameter, which can also be seen in Figure 2. As discussed earlier, the indirect-to-direct bandgap transition point of bulk $\text{Ge}_{1-x}\text{Sn}_x$ alloy is about $x = 0.086$, whereas for $\text{Ge}_{1-x}\text{Sn}_x$ NWs, the transition point x rises due to the quantum confinement effect. Let us move to Figure 3d with $x = 0.14$, $\text{Ge}_{1-x}\text{Sn}_x$ NWs becomes a direct-band-gap semiconductor completely whether D is 12 or 24 nm, which will lead to a large occupied proportion of the electron at the Γ -valley in Figure 3d even though the injected electron concentration Δn further decreases to 0.4–0.8 N_0 .

Figure 3. a) The proportion of the occupied electron concentration Δn_Γ at the Γ -valley to the total injected electron concentration Δn as a function of Δn with Sn content $x = 0.05$. N_0 represents the value $1 \times 10^{19} \text{ cm}^{-3}$. b-d) The same as (a), but for $x = 0.08, 0.11$, and 0.14 , respectively.

Before calculating the optical gain of $\text{Ge}_{1-x}\text{Sn}_x$ NWs, the energy difference $\Delta E_{e,01}^\Gamma$ and $\Delta E_{e,01}^L$ as functions of Sn content x and the diameter D between two lowest electron states at the minimum Γ -valley and the minimum L -valley are shown in Figure 4a,b, respectively. Obviously, $\Delta E_{e,01}^\Gamma$ and $\Delta E_{e,01}^L$ all increase slightly with increasing Sn content x when the diameter D is fixed. However, keeping Sn content x fixing, $\Delta E_{e,01}^\Gamma$ and $\Delta E_{e,01}^L$ all decrease substantially as the increase in the diameter D . Moreover, it can be found that $\Delta E_{e,01}^\Gamma$ is larger than $\Delta E_{e,01}^L$ if D and x are the same. Therefore, the eightfold degeneracy of each electron state at the L -valley and the small value $\Delta E_{e,01}^L$ determine that the quasi-Fermi energy level of the conduction band in $\text{Ge}_{1-x}\text{Sn}_x$ NWs mainly depends on the energies of the first few electron states at the L -valley. The optical gain $g(E)$ along z direction of $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $D = 12 \text{ nm}$ and $x = 0.08$ as a function of Δn is shown in Figure 5a. $g(E)$ can be calculated as^[22]

$$g(E) = \left[1 - \exp\left(\frac{E - \Delta F}{k_B T}\right) \right] \frac{\pi e^2 \hbar}{m_0^2 \epsilon_0 n_r c E} \sum_{n_c, n_v} \int_{BZ} \frac{dk_z}{2\pi S} \frac{\hbar/\tau}{\pi[(E_{eh} - E)^2 + (\hbar/\tau)^2]} |M_{n_c, n_v}|^2 f_{n_c}(k_z)(1 - f_{n_v}(k_z)) \quad (5)$$

where $f_{n_c}(k_z)$ and $1 - f_{n_v}(k_z)$ are the Fermi-Dirac distribution functions of the electron and hole, respectively. Meanwhile, during the calculation of the squared optical transition matrix element $|M_{n_c, n_v}|^2$, the optical transition selection rule of NWs from n_c th electron state to n_v th hole state is satisfied. We neglect the indirect-band-gap optical transition between the Γ -valley and the L -valley caused by phonon assistance, which is a second-order process.^[34]

Figure 4. a) The energy difference $\Delta E_{e,01}^\Gamma$ between two lowest electron states at the minimum Γ -valley as functions of Sn content x and the diameter D . b) The energy difference $\Delta E_{e,01}^L$ between two lowest electron states at the minimum L -valley as functions of Sn content x and the diameter D .

In Figure 5a, it can be seen that the optical gain begins to larger than zero from $\Delta n = N_0$, and there is only one peak in the figure as the increase in Δn . The peak gain value can increase to about 3000 cm^{-1} at the photon energy $E \approx 0.70 \text{ eV}$, which belongs to the infrared range. Through the analysis, the peak corresponds to the optical transition from the electron state $e_0^{1/2}$ to the hole state $h_0^{1/2}$, namely, $e_0^{1/2} \Rightarrow h_0^{1/2}$. As energy difference in bulk Ge between the direct-band-gap Γ -valley and indirect-band-gap L -valley is about 136 meV , the transparent injected electron concentration Δn of pure Ge NWs is about $4 N_0$,^[22] which is larger than that of $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $x = 0.08$ in Figure 5a. For $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $D = 18 \text{ nm}$, the optical gain is shown in Figure 5b. The peak gain value is about 2179.34 cm^{-1} at the photon energy $E \approx 0.64 \text{ eV}$ if Δn increases to $3 N_0$. In addition, another gain peak begins to appear, but it is not obvious. Figure 5c is the same as Figure 5b but for $D = 24 \text{ nm}$. Obviously, except the first peak, another peak will arise from $\Delta n = 2 N_0$, and this peak gain value can increase to about 1269.47 cm^{-1} at the photon energy $E \approx 0.657 \text{ eV}$, which is close to the first peak gain value 1561.77 cm^{-1} at $E \approx 0.612 \text{ eV}$. It can be analyzed that the second gain peak corresponds to the optical transitions $e_1^{1/2} \Rightarrow h_1^{1/2}$ and $e_0^{3/2} \Rightarrow h_1^{3/2}$, where the superscript $1/2$ and $3/2$ represent the total angular momentum projection along z axis of NWs.^[22] As we

Figure 5. a) The optical gain along z direction of $\text{Ge}_{1-x}\text{Sn}_x$ NWs as a function of Δn with $x = 0.08$ when $D = 12$ nm. b,c) The same as (a), but for $D = 18$ and 24 nm, respectively.

know, as the increase in the diameter, the electron and hole states become very dense, which may result in the appearance of more gain peaks. **Figure 6a** shows the same optical gain along z direction as Figure 5a but for $D = 12$ nm and $x = 0.11$. Compared with Figure 5a, two points should be emphasized in the figure. First, the transparent injected electron concentration decreases to about $0.6 N_0$, and the peak gain value is also about 3000 cm^{-1} when Δn decreases from $3 N_0$ in Figure 5a to $1.5 N_0$ in Figure 6a due to the further decrease in bulk ΔE_g^{bulk} of $\text{Ge}_{1-x}\text{Sn}_x$ alloy with $x = 0.11$; second, the optical gain spectra shows the obvious redshift in Figure 6a. Similarly, Figure 6b,c are the same as corresponding Figure 5b,c, respectively but for $x = 0.11$. It can be found that there are also two obvious gain peaks with $D = 24$ nm when $\Delta n = 1.5 N_0$ in Figure 6c, and they correspond to the same optical transitions as in Figure 5c.

The FCA loss of $\text{Ge}_{1-x}\text{Sn}_x$ NWs can be calculated via the following Drude-Lorentz equation^[35]

$$\alpha_f = \frac{e^3 \lambda^2}{4\pi^2 c^3 \epsilon_0 n_r} \left[\frac{N_e^\Gamma}{\mu_\Gamma (m_{\text{cl}}^*)^2} + \frac{N_e^L}{\mu_L (m_{\text{cl}}^*)^2} + \frac{N_h}{\mu_h (m_h^*)^2} \right] \quad (6)$$

where λ is the free space wavelength of $\text{Ge}_{1-x}\text{Sn}_x$ NWs, and m_{cl}^* and m_{cl}^* are the conductivity effective masses of $\text{Ge}_{1-x}\text{Sn}_x$ at the Γ -valley and L -valley, respectively. m_h^* is the heavy hole effective-mass for unstrained $\text{Ge}_{1-x}\text{Sn}_x$, and can be calculated by using two Luttinger parameters γ_1 and γ_2 of $\text{Ge}_{1-x}\text{Sn}_x$ ^[22,36] **Figure 7a** shows the peak gain along z direction, FCA loss and net peak gain of $\text{Ge}_{1-x}\text{Sn}_x$ NWs as a function of Δn when $D = 12$ nm and $x = 0.08$. We can see that FCA loss almost increase linearly with the increase in Δn , and will always below 1000 cm^{-1} even though Δn increases to $3 N_0$. Obviously, FCA loss becomes to be smaller than the corresponding peak gain value, and the net peak gain is positive from $\Delta n = 2 N_0$. In Figure 7b,c, the peak gain along z direction and FCA loss with $D = 18$ and 24 nm are presented, respectively. Although FCA loss in Figure 7b is slightly larger than that in Figure 7a, net peak gain in Figure 7b will become positive from $\Delta n = 1.5 N_0$. However, net peak gain decreases from about 2346.12 cm^{-1} in Figure 7a to about 1334.90 cm^{-1} in Figure 7b when Δn keeps $3 N_0$. Similarly, in Figure 7c, net peak gain is greater than zero from $\Delta n = 1.5 N_0$ and will further decrease to about 637.70 cm^{-1}

Figure 6. a) The optical gain along z direction of $\text{Ge}_{1-x}\text{Sn}_x$ NWs as a function of Δn with $x = 0.11$ when $D = 12$ nm. b,c) The same as (a), but for $D = 18$ and 24 nm, respectively.

Figure 7. a) The peak gain along z direction, FCA loss and net peak gain of $\text{Ge}_{1-x}\text{Sn}_x$ NWs as a function of Δn with $D = 12$ nm and $x = 0.08$. b,c) The same as (a), but for $D = 18$ and 24 nm, respectively. d) The peak gain along z direction, FCA loss, and net peak gain of $\text{Ge}_{1-x}\text{Sn}_x$ NWs as a function of Δn with $D = 12$ nm and $x = 0.11$. e,f) The same as (d), but for $D = 18$ and 24 nm, respectively.

even if Δn is $3 N_0$. When Sn content x increases from 0.08 to 0.11, the peak gain along z direction, FCA loss and net peak gain of $\text{Ge}_{1-x}\text{Sn}_x$ NWs with $D = 12$ nm as a function of Δn is shown in Figure 7d. Because of the decrease in Δn , FCA loss even becomes below 500 cm^{-1} when $\Delta n = 1.5 N_0$. Therefore, compared with Figure 7a, net peak gain will be improved. Figure 7e,f are the same as Figure 7d but for $D = 18$ and 24 nm, respectively. In these two figures, FCA loss are all below 500 cm^{-1} even though Δn increases to $1.5 N_0$ and the positive net peak gain is more easily obtained with small Δn . Therefore, according to above analysis about FCA loss and net peak gain, we can conclude that $\text{Ge}_{1-x}\text{Sn}_x$ NWs can be realized as lasers with the positive net peak gain whether the diameter is 12, 18 or 24 nm. While in ref. [22], the calculated results show that the positive net peak gain cannot be obtained for pure Ge NWs with large diameters even though the injected electron concentration Δn is in the range of $4\text{--}9 N_0$.

In summary, the electronic structures of $\text{Ge}_{1-x}\text{Sn}_x$ NWs at the Γ -valley and L -valley are calculated by using the effective-mass theory. Our results show that $\text{Ge}_{1-x}\text{Sn}_x$ NWs with large diameter and Sn content are easy to become the direct-band-gap semiconductor. With increasing Sn content, the proportion of the occupied electron concentration at the Γ -valley will increase substantially, which can enhance the light-emitting efficiency in $\text{Ge}_{1-x}\text{Sn}_x$ NW lasers. Meanwhile, the variation of the optical gain and FCA loss of $\text{Ge}_{1-x}\text{Sn}_x$ NWs with the diameter and injected

electron concentration are also studied, and it is found that a remarkable gain peak value can be obtained as the increase in Sn content even though the injected electron concentration decreases. Therefore, we can get a positive net peak gain in $\text{Ge}_{1-x}\text{Sn}_x$ NW lasers even at a diameter of 24 nm, which is different from the case of Ge NWs. Our theoretical studies can guide the practical applications of $\text{Ge}_{1-x}\text{Sn}_x$ NWs as the optoelectronic devices.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords

eight-band effective-mass theory, electronic structure, $\text{Ge}_{1-x}\text{Sn}_x$ nanowires, optical gain

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