Theoretical gain of strained $\text{GeSn}_{0.02}/\text{Ge}_{1-x-y}\text{Si}_x\text{Sn}_y$ quantum well laser

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Using effective-mass Hamiltonian model of semiconductors quantum well structures, we investigate the electronic structures of the Γ -conduction and L -conduction subbands of $\text{GeSn}/\text{GeSiSn}$ strained quantum well structure with an arbitrary composition. Our theoretical model suggests that the band structure could be widely modified to be type I, negative-gap or indirect-gap type II quantum well by changing the mole fraction of α -Sn and Si in the well and barrier layers, respectively. The optical gain spectrum in the type I quantum well system is calculated, taking into account the electrons leakage from the Γ -valley to L -valley of the conduction band. We found that by increasing the mole fraction of α -Sn in the barrier layer and not in the well layer, an increase in the tensile strain effect can significantly enhance the transition probability, and a decrease in Si composition in the barrier layer, which lowers the band edge of Γ -conduction subbands, also comes to a larger optical gain.

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I. INTRODUCTION

Silicon or germanium group IV semiconductor alloys containing Sn, which undergo indirect to direct band gap transitions, provide a wide opportunity for the integration of microelectronics with optical components into a single chip. It is well-known that bulk Si or Ge is an indirect-band-gap semiconductor, whose lowest-energy transition from valence to conduction bands involves a change in crystal momentum, whereas the gray tin structure is neither ideally semiconducting nor metallic.¹ These results suggest that perhaps one can combine the alloys containing only group IV elements wherein the difference in rows of the periodic table provides the contrast in optical transition probability. Most studied systems have been alloys of GeSn ,² GeSiSn ,³ and SiSn ⁴ systems. $\text{Ge}_{1-x}\text{Sn}_x$, which has a lower band gap than that of Ge (0.8 eV), is realized as the only one direct band gap material which is composed entirely of group IV elements. Thus, hybrid $\text{GeSn}/\text{GeSiSn}$ strained-layer heterostructures could possibly give exhibit to novel optical properties such as tunable narrow direct band gap, and could be very attractive for the detector and photovoltaic applications.

In this paper, we investigate the electronic structures and optical gain of a fully strained $\text{Ge}_{1-y}\text{Sn}_y/\text{Ge}_{1-x-y}\text{Si}_x\text{Sn}_y$ quantum well (QW) grown along [001] axis. Based on the eight-band effective-mass Hamiltonian model, the band structures in the Γ -valley are derived, including the interaction between the conduction and valence band, the spin-orbit coupling within the valence bands, and the deformation potential that describe the effects of strain on the electronic

bands.⁵ Taking into account the carrier occupation in both the Γ -valley and L -valley, we discuss the optical gain spectra with different mole fraction of α -Sn and Si composition in the barrier and well layers. The rest of the paper is organized as follows. In Sec. II, we present the theoretical model for the system being considered and introduce the optical gain calculation method. Our numerical results and discussion are given in Sec. III. Finally, we draw a brief conclusion in Sec. IV.

II. THEORETICAL MODEL

In this section, we use the effective-mass approximation to find the electron and hole energy levels at the Γ -valley and L -valley, respectively, and derive the theoretical model of the optical gain.

A. Band structures at Γ -valley

The Hamiltonian for strained QW semiconductor can be simply written as

$$H = H_k + V_{\Gamma}(z) + H_s, \quad (1)$$

where H_k is the kinetic eight-band effective-mass Hamiltonian including the interaction between the conduction and valence bands and the spin-orbit coupling within the valence bands. We adopt the second-order eight-band Hamiltonian as described by Kane,

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$$H_k = \frac{1}{2m_0} \begin{pmatrix} \alpha p^2 + 2m_0 E_g & & & & & & & \\ \frac{1}{\sqrt{2}} i p_0 p_- & -P_1 & & & & & & \\ -\frac{1}{\sqrt{6}} i p_0 p_+ & R^* & -P_2 & & & & & \\ -\frac{1}{\sqrt{3}} i p_0 p_+ & \sqrt{2} R^* & -\frac{1}{\sqrt{2}} (P_1 - P_2) & -\frac{1}{2} (P_1 + P_2) - 2m_0 \Delta_0 & & & & \\ 0 & 0 & -\sqrt{\frac{2}{3}} i p_0 p_z & \frac{1}{\sqrt{3}} i p_0 p_z & \alpha p^2 + 2m_0 E_g & & & \\ -\sqrt{\frac{2}{3}} i p_0 p_z & -Q^* & 0 & \sqrt{\frac{2}{3}} Q & \frac{1}{\sqrt{6}} i p_0 p_- & -P_2 & & \\ 0 & 0 & -Q^* & \frac{1}{\sqrt{2}} Q^* & \frac{1}{\sqrt{2}} i p_0 p_+ & -R^* & -P_1 & \\ \frac{1}{\sqrt{3}} i p_0 p_z & \frac{1}{\sqrt{2}} Q^* & -\sqrt{\frac{2}{3}} Q & 0 & \frac{1}{\sqrt{3}} i p_0 p_- & -\frac{1}{\sqrt{2}} (P_1 - P_2) & -\sqrt{2} R & -\frac{1}{2} (P_1 + P_2) - 2m_0 \Delta_0 \end{pmatrix}. \quad (2)$$

where

$$P_1 = (\gamma_1 + \gamma_2)(p_x^2 + p_y^2) + (\gamma_1 - 2\gamma_2)p_z, \quad (3a)$$

$$P_2 = (\gamma_1 - \gamma_2)(p_x^2 + p_y^2) + (\gamma_1 + 2\gamma_2)p_z, \quad (3b)$$

$$Q = -2\sqrt{3}\gamma_3 p_z(p_x - ip_y), \quad (3c)$$

$$R = \sqrt{3}[\gamma_2(p_x^2 - p_y^2) - 2i\gamma_3 p_x p_y], \quad (3d)$$

$$p_{\pm} = p_x \pm ip_y, \quad (3e)$$

$$p^2 = p_x^2 + p_y^2 + p_z^2. \quad (3f)$$

γ_1 , γ_2 , and γ_3 are the modified effective-mass parameters. They are related to the Luttinger parameters γ_i^L ($i=1, 2, 3$) as $\gamma_1 = \gamma_1^L - E_p/3E_g$, $\gamma_2 = \gamma_2^L - E_p/6E_g$, and $\gamma_3 = \gamma_3^L - E_p/6E_g$. E_g is the band gap and E_p is the Kane parameter that controls mixing of the valence and conduction bands, which is related to p_0 by $E_p = 2|\langle S|p_x|X \rangle|^2/m_0 = p_0^2/2m_0$ in Eq. (2).

The second term $V_{\Gamma}(z)$ is the intrinsic band offset without the contribution from the strain. The last term H_s in Eq. (1) is the strain-induced Hamiltonian. Hydrostatic and shear strain components are included by the same symmetry consideration and can be written as

$$H_s = \begin{pmatrix} a_c \epsilon & & & & & & & \\ -\frac{1}{\sqrt{2}} i p_0 p'_- & a_v \epsilon - b_v Q_E & & & & & & \\ \frac{1}{\sqrt{6}} i p_0 p'_+ & 0 & a_v \epsilon + b_v Q_E & & & & & \\ \frac{1}{\sqrt{3}} i p_0 p'_+ & 0 & -\sqrt{2} b_v Q_E & a_v \epsilon & & & & \\ 0 & 0 & \sqrt{\frac{2}{3}} i p_0 \epsilon_{zz} p_z & -\frac{1}{\sqrt{3}} i p_0 \epsilon_{zz} p_z & a_c \epsilon & & & \\ \sqrt{\frac{2}{3}} i p_0 \epsilon_{zz} p_z & 0 & 0 & 0 & -\frac{1}{\sqrt{6}} i p_0 p'_- & a_v \epsilon + b_v Q_E & & \\ 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} i p_0 p'_+ & 0 & a_v \epsilon - b_v Q_E & \\ -\frac{1}{\sqrt{3}} i p_0 \epsilon_{zz} p_z & 0 & 0 & 0 & -\frac{1}{\sqrt{3}} i p_0 p'_- & -\sqrt{2} b_v Q_E & 0 & a_v \epsilon \end{pmatrix}. \quad (4)$$

where

$$p'_\pm = \epsilon_{xx} p_x \pm i\epsilon_{yy} p_y, \quad (5a)$$

$$\epsilon = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz}, \quad (5b)$$

$$Q_E = \frac{1}{2}(2\epsilon_{zz} - \epsilon_{xx} - \epsilon_{yy}). \quad (5c)$$

$a_c(a_v)$ is the hydrostatic deformation potential of the Γ -conduction (valence) band, and b_v is the shear deformation potential of the valence band. ϵ_{xx} , ϵ_{yy} , and ϵ_{zz} are diagonal components of the strain tensor. We assume the strain of the barrier is completely relaxed, so that the lattice of the well layer is expanded by that of the barrier layer. For a [001] QW without the external stress, the three diagonal components of the strain tensor in the QW region are determined by the barrier and unstrained well lattice constants, a_b and a_w , as well as the QW elastic stiffness constants, C_{11} and C_{12}

$$\epsilon_{xx} = \epsilon_{yy} = \frac{a_b - a_w}{a_w}, \quad \epsilon_{zz} = -2\frac{C_{12}}{C_{11}}\epsilon_{xx}. \quad (6)$$

The set of basis states includes the s -like spin-up and spin-down conduction-band states, the fourfold p -like $J=3/2$ valence-band states, and twofold $J=1/2$ spin-orbit split-off valence-band states. The eight-dimensional electron and hole wave function of QW can be expressed as

$$\Psi_n(\mathbf{k}) = \sum_{j=1}^8 F_j(n, \mathbf{k}) u_j, \quad (7)$$

$$F_j(n, \mathbf{k}) = e^{i(k_x x + k_y y)} \sum_m a_j^{n,m} \frac{1}{\sqrt{L}} \exp\left[i\left(k_z + m\frac{2\pi}{L}\right)z\right], \quad (8)$$

where F_j is a slowly varying envelope function along z axis, and u_j are renormalized $|J, m_j\rangle$ Bloch states at Γ point. $L=l+d$ is the period of the QW and l and d are the width of the well and barrier layers, respectively. $a_j^{n,m}$ is the expansion coefficient. The Bloch basic functions are listed as follow

$$u_1 = |S\rangle\uparrow, \quad (9a)$$

$$u_2 = \frac{1}{\sqrt{2}}|X + iY\rangle\uparrow, \quad (9b)$$

$$u_3 = -\frac{1}{\sqrt{6}}|X - iY\rangle\uparrow - \sqrt{\frac{2}{3}}|Z\rangle\downarrow, \quad (9c)$$

$$u_4 = -\frac{1}{\sqrt{3}}|X - iY\rangle\uparrow + \frac{1}{\sqrt{3}}|Z\rangle\downarrow \quad (9d)$$

$$u_5 = |S\rangle\downarrow, \quad (9e)$$

$$u_6 = \frac{1}{\sqrt{6}}|X + iY\rangle\downarrow - \sqrt{\frac{2}{3}}|Z\rangle\uparrow, \quad (9f)$$

$$u_7 = \frac{1}{\sqrt{2}}|X - iY\rangle\downarrow, \quad (9g)$$

$$u_8 = \frac{1}{\sqrt{3}}|X + iY\rangle\downarrow + \frac{1}{\sqrt{3}}|Z\rangle\uparrow. \quad (9h)$$

B. Conduction band at L -valley

We calculate the band structure of the L -conduction valley under the effective-mass approximation. For a [001] QW, the eight equivalent L points in group IV semiconductors are degenerate. Due to the periodicity of the Brillouin zone, only four of them are independent, e.g., the [111] L -valley is identical to the $[\bar{1}\bar{1}\bar{1}]$ valley. Therefore, we can calculate only one particular valley for the sake of conciseness. For example, the Hamiltonian of [111] L -valley can be written as

$$H_L^{[111]} = \frac{\hbar^2 k_z^2}{2} \left(\frac{1}{3m_{l,L}} + \frac{2}{3m_{t,L}} \right) + \frac{\sqrt{2}\hbar^2 k_1 k_z}{3} \left(\frac{1}{m_{l,L}} - \frac{1}{m_{t,L}} \right) + \frac{\hbar^2 k_1^2}{2} \left(\frac{2}{3m_{l,L}} + \frac{1}{3m_{t,L}} \right) + \frac{\hbar^2 k_2^2}{2m_{t,L}} + V_L(z) + a_L \epsilon, \quad (10)$$

where $k_1 = (k_x + k_y - 2\pi/a)/\sqrt{2}$ and $k_2 = (-k_x + k_y)/\sqrt{2}$. $m_{l,L}$ and $m_{t,L}$ are the longitudinal and transverse effective masses along [111] direction. k_1 (along [110] direction) and k_2 (along $[\bar{1}\bar{1}0]$ direction) are wave vectors relative to the minimal point of the [111] L -valley, e.g., $(\pi/a, \pi/a)$, where a is the in-plane lattice constant of the QW material. $V_L(z)$ and $a_L \epsilon$ in Eq. (10) are the intrinsic band offset and hydrostatic deformation potential of the [111] L -valley, respectively. Then the energy dispersion relation of the [111] L -valley conduction band can be obtained by solving the eigenfunction with a similar envelope wave function $\chi_n^{[111]} = F_L(n, \mathbf{k}) v_L$, where v_L is the Bloch states at L point.

C. Carrier density in conduction and valence subbands

Using the charge neutrality condition when the electron and hole densities n_e and n_h are both the same as the injected carrier density $n = n_e = n_h$, we can obtain the quasi-Fermi levels. Since the interaction between the valence and conduction bands has caused the energy dispersion curves to be nonparabolic, the quasi-Fermi levels should be determined from the integration of the two-dimensional density of states in QW instead of analytical calculation for parabolic energy subbands. The carrier density by numerical integration over the k -space is

$$n_e = \sum_n \int \frac{dk_x dk_y}{4\pi^2 l} \frac{1}{\exp\left(\frac{E_n^\Gamma - E_{f_c}}{k_B T}\right) + 1} + \sum_n 8 \int \frac{dk_x dk_y}{4\pi^2 l} \frac{1}{\exp\left(\frac{E_n^L - E_{f_c}}{k_B T}\right) + 1} \quad (11)$$

for electrons, and

$$n_h = \sum_{\sigma, m} \int \frac{dk_x dk_y}{4\pi^2 l} \frac{1}{\exp\left(\frac{E_{f_v} - E_m^\sigma}{k_B T}\right) + 1} \quad (12)$$

for holes. n and m are indices of the conduction and valence subbands, and σ runs over all the six valence bands. A factor of 8 is included in the summation of L -conduction subbands due to the spin degeneracy of four equivalent L -valleys. E_{f_c} and E_{f_v} are electron and hole quasi-Fermi levels, respectively, and they are determined self-consistently from Eqs. (11) and (12). k_B is the Boltzmann's constant and T is the temperature.

D. Optical gain

According to the relationship between spontaneous emission and gain, we calculate the optical gain by using an indirect technique.^{5,6} The optical gain can be written as

$$g(E) = \left[1 - \exp\left(\frac{E - \Delta F}{k_B T}\right) \right] \frac{\pi^2 c^2 \hbar^3}{n_r^2 E^2} R_{sp}(E) \quad (13)$$

in which spontaneous emission rate

$$R_{sp}(E) = \frac{n_r E}{\pi \epsilon_0 \hbar^2 c^3 l} \left(\frac{e}{m_0} \right)^2 \sum_{n_c, n_v} \int \frac{dk_x dk_y}{4\pi^2} Q^{n_c, n_v} f_{n_c} (1 - f_{n_v}) \frac{1}{\pi (E_{eh} - E)^2 + (\hbar/\tau)^2}, \quad (14)$$

where $\Delta F = E_{f_c} - E_{f_v}$ is the quasi-Fermi level separation, E is the photon energy, n_r is the refractive index, and τ is the intraband relaxation time. The Fermi-Dirac distributions for the electrons in the conduction band and the valence band are f_{n_c} and f_{n_v} , respectively. The f_n is defined as

$$f_n = \left[\exp\left(\frac{E_n - E_f}{k_B T}\right) + 1 \right]^{-1}. \quad (15)$$

Q^{n_c, n_v} in Eq. (14) represents the squared optical transition matrix elements for transitions between the valence subbands and the conduction subbands at Γ point.⁵

$$Q_i^{n_c, n_v} = \frac{2}{m_0} |\langle \Psi_{n_c} | \hat{\epsilon} \cdot \mathbf{p} | \Psi_{n_v} \rangle|^2, \quad i = x, y, z, \quad (16)$$

where $\hat{\epsilon}$ is the unit vector in the direction of the electric field, $\mathbf{p}$ is the momentum operator, and $\Psi_{n_c}(\Psi_{n_v})$ is the real electron and hole wave function. Substituting Eqs. (7) and (8) into Eq. (16), we obtain the expression for squared optical transition matrix elements in X , Y , and Z directions as

$$Q_{x\uparrow}^{n_c, n_v} = \frac{2P_0^2}{m_0} \left| \sum_m \left(\frac{1}{\sqrt{2}} a_2^m - \frac{1}{\sqrt{6}} a_3^m - \frac{1}{\sqrt{3}} a_4^m \right) a_1^{m*} \right|^2, \quad (17a)$$

$$Q_{x\downarrow}^{n_c, n_v} = \frac{2P_0^2}{m_0} \left| \sum_m \left(\frac{1}{\sqrt{6}} a_6^m + \frac{1}{\sqrt{2}} a_7^m + \frac{1}{\sqrt{3}} a_8^m \right) a_5^{m*} \right|^2, \quad (17b)$$

$$Q_{y\uparrow}^{n_c, n_v} = \frac{2P_0^2}{m_0} \left| \sum_m \left(\frac{1}{\sqrt{2}} a_2^m + \frac{1}{\sqrt{6}} a_3^m + \frac{1}{\sqrt{3}} a_4^m \right) a_1^{m*} \right|^2, \quad (17c)$$

TABLE I. The band parameters at 300 K for bulk α -Sn, Ge, and Si in the actual calculation (Ref. 11).

Parameter	Sn	Ge	Si
a (Å)	6.4892	5.6573	5.4307
m_c (m_0)	-0.058	0.038	0.528
$m_{l,L}$ (m_0)	0.4072	1.57	1.659
$m_{t,L}$ (m_0)	0.0204	0.0807	0.133
γ_1	-15	13.38	4.22
γ_2	-11.45	4.24	0.39
γ_3	-8.55	5.69	1.44
E_p (eV)	24.0	26.3	21.6
$E_{g,\Gamma}$ (eV)	-0.413	0.7985	4.185
$E_{g,L}$ (eV)	0.092	0.664	1.65
Δ_0 (eV)	0.8	0.29	0.044
$\Delta E_{v,av}$ (eV)	0.69	0	-0.47
a_c (eV)	-5.33 ^a	-8.24	1.98
a_v (eV)	1.55 ^a	1.24	2.46
a_L (eV)	-0.342 ^b	-1.54	-0.66
b_v (eV)	-2.7	-2.9	-2.1
C_{11} (10 GPa)	6.9	12.853	16.577
C_{12} (10 GPa)	2.9	4.826	6.393
n_r	4.90	4.02	3.45

^aReference 9.

^bPresent work which is given in Appendix.

$$Q_{y\downarrow}^{n_c, n_v} = \frac{2P_0^2}{m_0} \left| \sum_m \left(\frac{1}{\sqrt{6}} a_6^m - \frac{1}{\sqrt{2}} a_7^m + \frac{1}{\sqrt{3}} a_8^m \right) a_5^{m*} \right|^2, \quad (17d)$$

$$Q_{z\uparrow}^{n_c, n_v} = \frac{2P_0^2}{m_0} \left| \sum_m \left(-\sqrt{\frac{2}{3}} a_6^m + \frac{1}{\sqrt{3}} a_8^m \right) a_1^{m*} \right|^2, \quad (17e)$$

$$Q_{z\downarrow}^{n_c, n_v} = \frac{2P_0^2}{m_0} \left| \sum_m \left(-\sqrt{\frac{2}{3}} a_3^m + \frac{1}{\sqrt{3}} a_4^m \right) a_5^{m*} \right|^2, \quad (17f)$$

and

$$Q_i^{n_c, n_v} = Q_{i\uparrow}^{n_c, n_v} + Q_{i\downarrow}^{n_c, n_v}, \quad i = x, y, z, \quad (18)$$

where $P_0^2 = |\langle S | p_x | X \rangle|^2 = |\langle S | p_y | Y \rangle|^2 = |\langle S | p_z | Z \rangle|^2$. In our calculation, we average $Q_{x\uparrow}^{n_c, n_v}$ and $Q_{y\uparrow}^{n_c, n_v}$ to obtain $Q_{xy}^{n_c, n_v}$ for the TE model, and $Q_{z\uparrow}^{n_c, n_v}$ alone indicates the TM model. Note that the highest valence band is light hole (LH)-like; the TM gain will be significant.

III. RESULTS AND DISCUSSIONS

In this section, we calculate the electronic structures and optical gain spectrum of the strained $\text{Ge}_{1-y}\text{Sn}_y/\text{Ge}_{1-x-y}\text{Si}_x\text{Sn}_y$ QW. All the other parameters are calculated using a simple linear average between Ge, Si, and α -Sn, whose values are listed in Table I for the QW and barrier materials, except the band-gap energies for semiconductor alloys. We use the band-gap energy included the bowing effect and the strain-dependent spin-orbit energy following Chandrasekhar and Pollak's approach.⁷ Alloy band gap E_g at 300 K of $\text{Ge}_{1-y}\text{Sn}_y$ and $\text{Ge}_{1-x-y}\text{Si}_x\text{Sn}_y$ at Γ and L points could be fitted to the following form:

$$E_{g,\sigma}^{\text{GeSn}} = E_{g,\sigma}^{\text{Ge}}(1-y) + E_{g,\sigma}^{\text{Sn}}y - b_{\sigma}^{\text{GeSn}}y(1-y), \quad (19)$$

FIG. 1. (Color online) The band gap of a fully strained $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{1-x-y}/\text{Si}_x\text{Sn}_{y'}$ QW with relaxed barrier layers.

$$E_{g,\sigma}^{\text{GeSiSn}} = E_{g,\sigma}^{\text{Ge}}(1-x-y') + E_{g,\sigma}^{\text{Si}}x + E_{g,\sigma}^{\text{Sn}}y' - b_{\sigma}^{\text{GeSi}}x(1-x-y') - b_{\sigma}^{\text{GeSn}}y'(1-x-y') - b_{\sigma}^{\text{SiSn}}xy', \quad (20)$$

$\sigma = \Gamma, L$. For the value of fitted alloy bowing factors, we use $b_{\Gamma}^{\text{GeSi}} = 0.14$, $b_{\Gamma}^{\text{SiSn}} = 3.05$,⁸ $b_{\Gamma}^{\text{GeSn}} = 2.55$, $b_L^{\text{GeSn}} = 0.89$,⁹ $b_L^{\text{GeSi}} = 0.335$, and $b_L^{\text{SiSn}} = 3.124$ ¹⁰ for the recent measures for these alloys. We consider a $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{1-x-y}/\text{Si}_x\text{Sn}_{y'}$ QW. The positive energy-gap value of direct-gap semiconductor QW is depicted in Fig. 1. The colored regions in the figure indicate the compositions for which the QW is of type I heterostructure corresponding to both Γ electrons and holes confined in the well layer. The band-gap energy is up to 0.3 eV, and can be tuned to negative value with the increasing α -Sn composition y' , depicted at right side of the figure. It indicates that semimetal properties would be found in heavy dropped α -Sn QW construction. At the left edge of the figure, which corresponds to the light Sn dropping case, the lowest conduction band edge is located at the L -conduction valley in the barrier layer. As the decreasing Si composition x , it becomes a direct type II QW structure. Therefore, the concentration of QW and barrier layer components should greatly influence the locations of the carriers, and their optical properties. When the concentration of α -Sn in the well layer is increased, the optical positive area (colored region in the Fig. 1) becomes smaller even more.

A. Electron and hole levels

We consider a $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{0.68}\text{Si}_{0.1}\text{Sn}_{0.22}$ QW structure, whose mole fraction parameters in the barrier layer are selected in the colored region, with a width of 7 nm and a period of 20 nm. The tensile strain of QW $\epsilon_{xx} = 0.0253$, and it would be expected to be of type I heterostructure. The zero energy is set to the top of valence band of unstrained well layer. The lowest electron and hole levels near band gap are shown in Figs. 2(a) and 2(b). All the energy levels depicted in the figures are twofold degenerate. Due to the interaction between conduction and valence bands, the energy-wave vector dispersion relation of electron levels is nonparabolic. The strain effect separates the heavy hole (HH) and LH sub-

FIG. 2. (a) The lowest electron and (b) hole subbands of a fully strained $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{0.68}\text{Si}_{0.1}\text{Sn}_{0.22}$ QW at the Γ -valley.

bands. The LH subbands are pushed to the higher energy side and turn out to be the top of valence bands. The band gap of this QW is 0.37 eV, equivalent to a cutoff wavelength of about $3.35 \mu\text{m}$. Figure 3 shows the electron levels of $[111]$ L -conduction band as a function of the wave vectors along $[110]$ and $[\bar{1}10]$ direction. The smooth dispersion relation in the L -valley reflects a large effective mass. As all the levels in the L -valley are eightfold degenerate, it results in a high density of states. Therefore, there is significant carrier leakage from the Γ -valley to L -valley, and it is expected that the optical transition could be greatly reduced. It is very interesting to find band bending at higher energy levels at the L -valley along $[110]$ direction. This bending behavior is because the effect of effective-mass anisotropy and the wave vector k_1 is neither along the longitudinal nor along transverse axes of ellipsoidal constant energy surface for L -valley

FIG. 3. The lowest electron subbands at the $[111]$ L -valley.

FIG. 4. The squared optical transition matrix elements for TE and TM model transition from the lowest conduction subband to the valence subband as a function of k along the $[100]$ and $[110]$ directions.

electrons, which is expressed as $k_1 \cdot k_z$ terms in $H_L^{[111]}$. As the quantum number increases, the band bends further. Considering the energy difference between the ground state and first-excited state of L -conduction subband is 32 meV at $k_1 = k_2 = 0$ point, which is larger than Boltzmann energy $k_B T = 25$ meV at 300 K, we suppose that the electrons seldom occupy the excited states with a moderate injected carrier density.

B. Optical gain

The squared optical transition matrix elements for TE and TM mode transitions from the first LH energy level to the first conduction subband energy level as a function of k along the $[100]$ and $[110]$ directions are shown in Fig. 4. The transition from valence band to conduction band follows the selection rule $\Delta n = 0$ the Γ point. According to Eq. (17), the contribution from electron to spin-orbit split-off hole is mainly the same for each squared optical transition matrix elements. As the spin-orbit split-off hole subband is much lower than the top valence band, the corresponding transition is very weak. The squared optical transition matrix elements for TE model are the sum of the major contribution from electron to HH transition and the minor contribution from electron to light hole transition. For the TM model, the contribution comes from the electron to light hole transition only. Because the ground hole state is light hole state [Fig. 2(b)], the optical gain of the TM model is much larger than that of the TE model.

Figure 5(a) shows the optical gain spectra with and without the inclusion of the conduction subbands in the L -valley at carrier density $n = 6 \times 10^{18} \text{ cm}^{-3}$. In our calculation, we set the intraband relaxation time $\tau = 0.0658 \text{ ps}$ and the temperature $T = 300 \text{ K}$. The TM polarized optical gain is higher than the TE model. For comparison, in Fig. 5(c) we plot the optical gain spectra of $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{0.725}\text{Si}_{0.1}\text{Sn}_{0.175}$ QW, which should be of type II from Fig. 1, at the same carrier density. As most of the electrons are confined in the L -conduction valley in the barrier layer, which results in the very weak overlap of electron and hole wave functions, the optical gain almost disappears. If we neglected the leakage of the carriers to the L -valley, where all the carriers accumu-

FIG. 5. (a) The optical gain spectra of $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{0.68}\text{Si}_{0.1}\text{Sn}_{0.22}$ QW with and without the inclusion of L -conduction subbands. (b) The carrier densities of Γ -conduction and L -conduction valleys as a function of the total electronic density. (c) The gain spectra of $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{0.725}\text{Si}_{0.1}\text{Sn}_{0.175}$ QW at the same injected carrier density.

lated in the Γ -conduction subbands, the optical gain increases significantly which is plotted in Fig. 5(a) with dotted lines. The electron densities of Γ -conduction subbands and L -conduction subbands as functions of the total carrier density is shown in Fig. 5(b). It represents that the occupation of the L -conduction valley is much more significant than that in the Γ -conduction valley because of lower energy levels and high degeneracy of electrons in the L -conduction valley. To reduce this unwanted effect from the L -conduction valley, one can increase the Sn mole fraction in the well layer that may lower the band edge of the Γ -conduction valley due to the negative band gap of α -Sn. However, it also suggests that an increase in the tensile strain effect may significantly increase the transition probability by changing the composition of the barrier alloy. Therefore the compositions at the barrier and well layers need to be well understood and carefully designed so that larger optical gain may be maintained.

The results of the calculated TM gain spectra for various Si and Sn mole fraction in barrier layer are shown in Figs. 6(a) and 6(b), respectively. In Fig. 6(a) we plotted curves for three selected Si mole fraction values for comparison. As the Si concentration decreases, the maximum for TM gain increases and the corresponding photon energy decreases. In the same way, we also plotted curves for three selected Sn mole fraction values in Fig. 6(b). As the Sn concentration increases, the maximum TM gain increases and the corre-

FIG. 6. TM gain spectra of (a) $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{0.78-x}\text{Si}_{0.22}$ and (b) $\text{Ge}_{0.98}\text{Sn}_{0.02}/\text{Ge}_{0.9-y}\text{Si}_{0.1}\text{Sn}_{0.22}$ QW structures at various mole fractions in the barrier layer.

sponding photon energy decreases, which confirms a smaller band-gap energy shown in Fig. 1. All the composition parameters are selected in the colored region in Fig. 1 for which the band gap is direct and localized in the well layer. With either decreasing Si or increasing Sn composition in the barrier layer, the lattice constant becomes larger and it makes an increase tensile strain in QW layer.

Figure 7 shows the TM gain spectra of $\text{Ge}_{1-y}\text{Sn}_y/\text{Ge}_{0.68}\text{Si}_{0.1}\text{Sn}_{0.22}$ QW structures at several values of Sn mole fraction in the well layer. We find that the maximum TM gain decreases with the increasing Sn composition. It is because that the lattice constant becomes larger and the tensile strain is reduced due to the decreasing of lattice constant difference between the barrier and well layers. Therefore, the maximum of optical gain decreases correspondingly. Meanwhile, both the Γ -conduction band and L -conduction band

FIG. 7. TM gain spectra of $\text{Ge}_{1-y}\text{Sn}_y/\text{Ge}_{0.68}\text{Si}_{0.1}\text{Sn}_{0.22}$ QW structures at various Sn mole fractions in the well layer. In the inset of the figure, we have plotted the band-gap energy difference between the L -valley and Γ -valley in the QW layer as a function of Sn mole fraction y .

are tending downward with the increasing Sn composition in the well layer. The band-gap energy difference between the L -valley and Γ -valley decrease with increasing Sn mole fraction, as depicted in the inset of Fig. 7. It represents that more carriers transfer from Γ -conduction valleys to the L -conduction valley as the Sn mole fraction increases, and the optical gain should be reduced even more. From both points of view, we predict that an increase in Sn mole fraction in the well region could lower the electron occupation of Γ -conduction states, which contribute to the optical gain at the same injected carrier density level.

IV. CONCLUSION

In summary, we have estimated the optical gain characteristics of a strain-induced $\text{Ge}_{1-y}\text{Sn}_y/\text{Ge}_{1-x-y'}\text{Si}_x\text{Sn}_{y'}$ 7 nm QW at specific α -Sn mole fraction in the well, based on the eight-band Hamiltonian in combination with a finite band offset model. By modifying the mole fraction of α -Sn and Si in the well and barrier layer, respectively, the theoretical calculation suggests that the conduction and valence band edge are shifted and result in the type I, negative-gap or indirect-gap type II QW structure. The variations in gain spectra with α -Sn and Si concentrations in well and barrier layers are calculated in details. With the increasing the mole fraction of α -Sn in barrier layer not in well layer, the tensile strain in the well layer increase, and the positive optical gain could be found in such systems, which are attractive from the points of view of both basic research and technological applications in a foreseeable future.

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APPENDIX

In this work, the absolute deformation potential (ADP) of zinc-blende Si, Ge, and Sn are calculated using the density functional theory within the general gradient approximation for the exchange-correlation potential as implemented in the Vienna *ab initio* simulation package code. We use the projector-augmented-wave pseudopotentials. The cutoff energy for plane wave expansion is 350 eV in all calculations. All atoms in the cell are fully relaxed until the forces are converged to better than 0.01 eV/Å. An $11 \times 11 \times 11$ Monkhorst-Pack k -point mesh is used for the Brillouin zone integration. The equilibrium lattice constants of bulk Si, Ge, and Sn are determined by performing a least-squares fit to the Murnaghan equation

$$E(V) = \frac{B_0 V}{B'_0 (B' - 1)} \left[B' \left(1 - \frac{V_0}{V} \right) + \left(\frac{V_0}{V} \right)^{B'_0} - 1 \right] + E(V_0), \quad (\text{A1})$$

where B_0 is the bulk modulus, $E(V_0)$ is the cohesive energy (when referenced to the proper energy of the isolated atom), B'_0 is pressure derivative of the bulk modulus, and V_0 is the equilibrium volume. The optimized results are 5.468, 5.779, and 6.648 for Si, Ge, and Sn, respectively. The ADPs are

calculated using the lattice harmonic expansion approach.

- ¹M. L. Cohen and J. R. Chelikowsky, *Electronic Structure and Optical Properties of Semiconductors* (Springer, Berlin, 1988).
- ²M. Bauer, C. Ritter, P. A. Crozier, J. Ren, J. Menendez, G. Wolf, and J. Kouvetakis, *Appl. Phys. Lett.* **83**, 2163 (2003).
- ³P. Aella, C. Cook, J. Tolle, S. Zollner, A. V. G. Chizmeshya, and J. Kouvetakis, *Appl. Phys. Lett.* **84**, 888 (2004).
- ⁴J. Tolle, A. V. G. Chizmeshya, Y. Y. Fang, J. Kouvetakis, V. R. D'Costa, C. W. Hu, J. Menendez, and I. S. T. Tsong, *Appl. Phys. Lett.* **89**, 231924 (2006).
- ⁵S. T. Ng, W. J. Fan, Y. X. Dang, and S. F. Yoon, *Phys. Rev. B* **72**, 115341 (2005).
- ⁶J. Minch, S. H. Park, T. Keating, and S. L. Chuang, *IEEE J. Quantum Electron.* **35**, 771 (1999).
- ⁷M. Chandrasekhar and F. H. Pollak, *Phys. Rev. B* **15**, 2127 (1977).
- ⁸V. R. D'Costa, C. S. Cook, J. Menendez, J. Tolle, J. Kouvetakis, and J. Zollner, *Solid State Commun.* **138**, 309 (2006).
- ⁹W. J. Yin, X. G. Gong, and S. H. Wei, *Phys. Rev. B* **78**, 161203 (2008).
- ¹⁰P. Moontragoon, Z. Ikonić, and P. Harrison, *Semicond. Sci. Technol.* **22**, 742 (2007).
- ¹¹S. S. Chang and S. L. Chuang, *IEEE J. Quantum Electron.* **43**, 249 (2007).