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Tensile-strain and doping enhanced direct bandgap optical transition of n^+ doped Ge/GeSi quantum wells

W. J. Fan^{a)}
 NOVITAS, Nanoelectronics Centre of Excellence, School of Electrical and Electronic Engineering,
 Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798

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Band structures of tensile strained and n^+ doped Ge/GeSi quantum wells (QWs) are calculated by multiple-band $k \cdot p$ method. The energy dispersion curves of the Γ and L conduction subbands are obtained. The effects of tensile strain and n^+ doping in Ge on direct bandgap optical gain and spontaneous radiative recombination rate spectra are investigated including the electron leakage from Γ to L conduction subbands. Our results show that the optical gain and spontaneous radiative recombination rate can be significantly increased with the tensile strain, n -type doping concentration, and injection carrier density in the Ge QW. The free carrier absorption is calculated and cannot be ignored because of the heavily doped Ge. The pure TM mode polarized net optical gain up to 1153 cm^{-1} can be achieved for the $\text{Ge}/\text{Ge}_{0.986}\text{Si}_{0.014}$ QW with tensile strain of 1.61% and n -type doping concentration of $30 \times 10^{18} \text{ cm}^{-3}$. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4831750>]

I. INTRODUCTION

Ge-on-Si has received great attention because it is a promising candidate for monolithic laser on Si platform and its fabrication is compatible with CMOS process.¹ Although Ge is an indirect band gap semiconductor, its L conduction band edge is just below Γ conduction band edge 136 meV only. So, Ge is called as a pseudo-direct band gap semiconductor.² And, the direct band gap of Ge is 0.8 eV, which exactly matches the $1.55 \mu\text{m}$ optical fiber windows. These unique features of Ge make it a potential candidate for Si-based fiber laser through proper bandgap engineering.³ Recently, both optically^{4,5} and electrically⁶ bumped room temperature multimode lasers based on n^+ doped and tensile strained Ge have been demonstrated.⁷ However, the lasing threshold is still quite high at about 280 kA/cm^2 , and the operation is still pulse not CW. In order to improve Ge laser performance, a Ge quantum well (QW) structure can be used to decrease the threshold current density due to the quantum confinement effect.

In this paper, we will calculate the band structures of n^+ doped and tensile strained Ge/GeSi QWs using the multiple-band $k \cdot p$ method. A single band effective mass Hamiltonian will be used to calculate the L conduction subbands in order to consider the electron leakage from Γ to L conduction subbands. And, the optical gain and spontaneous radiative recombination rate spectra will be obtained. At higher carrier concentration in Ge well, the free carrier absorption (FCA) has to be taken into account. And, the net gain will be calculated.

II. CALCULATION METHOD

A lot of 6 band $k \cdot p$ calculations have been performed in the strained bulk Ge and Ge QW.^{8,9} However, the direct

bandgap of Ge is about 0.8 eV only, the interaction between the conduction and valence bands should be included in the band structure calculations. So, the 8 band $k \cdot p$ or even more band $k \cdot p$ method, such as the 30 band $k \cdot p$,^{10,11} should be applied for the more accurate results. The subband energy dispersion curves near the Γ point of the [001]-oriented Ge/GeSi strained QWs can be calculated by using a 10-band $k \cdot p$ method which is described in detail in our previous work.¹² The nitrogen level and coupling coefficient can be set to 3000 meV and zero, respectively, to exclude the nitrogen level in our concerned energy range. This method is equivalent to degrade the 10 band $k \cdot p$ method to the 8 band $k \cdot p$ method.¹³ For the L conduction subbands, the Hamiltonian can be written by^{9,14}

$$\begin{aligned}
 H_L^{[111]} = & -\frac{\hbar^2}{2} \frac{\partial}{\partial z} \left(\frac{1}{3m_{l,L}} + \frac{2}{3m_{t,L}} \right) \frac{\partial}{\partial z} - i \frac{\sqrt{2}\hbar^2 k_1}{6} \\
 & \times \left[\frac{\partial}{\partial z} \left(\frac{1}{m_{l,L}} - \frac{1}{m_{t,L}} \right) + \left(\frac{1}{m_{l,L}} - \frac{1}{m_{t,L}} \right) \frac{\partial}{\partial z} \right] \\
 & + \left(\frac{2}{3m_{l,L}} + \frac{1}{3m_{t,L}} \right) \frac{\hbar^2 k_1^2}{2} + \frac{\hbar^2 k_2^2}{2m_{t,L}} + V^{[111]}(z) \\
 & + V_e^{[111]}(z),
 \end{aligned} \quad (1)$$

where

$$\begin{aligned}
 V_e^{[111]}(z) &= a_L(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}), \\
 k_1 &= \frac{1}{\sqrt{2}} \left(k_x + k_y - \frac{2\pi}{a} \right), \\
 k_2 &= \frac{1}{\sqrt{2}} (-k_x + k_y),
 \end{aligned} \quad (2)$$

$m_{l,L}$ and $m_{t,L}$ are the longitudinal and transverse effective masses along the [111] direction. The wave vector k_l is along [110] direction and k_2 is along [-110] direction. a is the in-plane lattice constant of well material. $V^{[111]}(z)$ and $V_e^{[111]}(z)$

^{a)}ewjfan@ntu.edu.sg

are the unstrained potential profile and the strain-induced energy shift for the L-conduction band edge, respectively. a_L is the hydrostatic deformation potential of the L-valley. ε_{xx} and ε_{yy} are the in-plane strain. $\varepsilon_{zz} = -2c_{12}/c_{11}\varepsilon_{xx}$ is the strain in the perpendicular direction. c_{11} and c_{12} are elastic stiffness coefficients.

The direct band gap optical gain can be calculated by^{15,16}

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

where $\Delta F = E_{fc} - E_{fv}$ is the quasi-Fermi levels separation. E_{fc} and E_{fv} are the electron and hole quasi-Fermi level in the conduction and valence band, respectively. k_B is the Boltzmann constant, T is the temperature, n is the refractive index, c is the light velocity. R_{sp} is the spontaneous radiative recombination rate in Refs. 15 and 16.

The FCA can be significant for the n^+ doped Ge and can be calculated by^{3,17}

$$\alpha_f = \frac{e^3 \lambda^2}{4\pi^2 c^3 \varepsilon_0 n} \left[\frac{n_\Gamma}{\mu_\Gamma (m_{c\Gamma}^*)^2} + \frac{n_L}{\mu_L (m_{cL}^*)^2} + \frac{p}{\mu_h (m_{ch}^*)^2} \right], \quad (4)$$

where e is the electronic charge, λ is the free space wavelength, n is the refractive index, ε_0 is the permittivity of free space. c is the speed of light in free space. n_Γ and n_L are the electron concentrations in the Γ and L valleys, respectively. p is the hole concentration. $m_{c\Gamma}^*$, m_{cL}^* , and m_{ch}^* are the conductivity effective masses of Γ valley electron, L valley electron, and hole, respectively. Because the Γ valley electron effective mass is isotropy, $m_{c\Gamma}^*$ is equal to m_Γ^* . Here, m_Γ^* is the band effective mass of electron in the Γ valley. However, the effective mass of electron in the L valley is anisotropy, its conductivity effective mass and band effective mass's relationship is given by

$$m_{cL}^* = \frac{3}{\frac{1}{m_{lL}^*} + \frac{2}{m_{tL}^*}}, \quad (5)$$

where m_{lL}^* and m_{tL}^* are the longitudinal and transverse band effective masses of electrons in the L valley. For the hole effective mass, generally it is anisotropy. However, for the tensile strain Ge, the top of valence band is light hole band and its effective mass is weakly anisotropy at smaller k range. As a reasonable approximation, one can assume the light hole conductivity effective mass is same as its band effective mass and can calculate it using the axial approximation¹⁸

$$m_{ch}^* \approx \frac{1}{\gamma_1 + \gamma_2 + \gamma_3}, \quad (6)$$

where γ_1 , γ_2 , and γ_3 are the Luttinger parameters. μ_Γ and μ_L are the electron mobilities in the Γ and L valleys, respectively. And μ_h is the light hole mobility. The electron mobilities in the L valleys are given by^{19,20}

$$\mu_L = \frac{3900}{1 + \sqrt{n_L \times 10^{-17}}}, \quad (7)$$

where μ_L is in the unit of $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ and n_L is in the unit of cm^{-3} . Assuming that the scattering times of electrons in the Γ and L valleys are the same in Ref. 3, the electron mobility in the Γ valleys is estimated by $\mu_\Gamma = \frac{m_{cL}^*}{m_{c\Gamma}^*} \mu_L$. And the hole mobility of Ge is given by²¹

$$\mu_h = \frac{1900}{1 + \sqrt{p \times 2.1 \times 10^{-17}}}, \quad (8)$$

where μ_h is in the unit of $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ and p is in the unit of cm^{-3} .

III. RESULTS AND DISCUSSIONS

The well and barrier widths of the studied Ge/ $\text{Ge}_{0.986}\text{Si}_{0.014}$ QWs are fixed at 112 Å and 85 Å, respectively, same as those in Ref. 22 for comparison.²² The band parameters used for the calculations are taken from Refs. 9 and 14, and are listed in Table I.²³ The bowing effect is taken into consideration in the GeSi alloy band gap calculation. The band gap of $\text{Ge}_x\text{Si}_{1-x}$ at Γ point is given by¹⁴

$$E_g^{\Gamma, \text{GeSi}} (\text{eV}) = 0.7985x + 4.185(1-x) - 0.14x(1-x). \quad (9)$$

The band gap of $\text{Ge}_x\text{Si}_{1-x}$ at L point is given by¹⁴

$$E_g^{L, \text{GeSi}} (\text{eV}) = 0.664x + 1.65(1-x) - 0.335x(1-x). \quad (10)$$

The band lineups of three Ge/ $\text{Ge}_{0.986}\text{Si}_{0.014}$ QWs with different tensile strains of 0.13%, 1.61%, and 2% are shown in Fig. 1. The energy zero point is set at the average energy level of unstrained Ge valance bands. The band lineups show that the QWs are type I. For Ge grown on Si, the stain in Ge is traditionally compressive strain. However, under special growth and fabrication condition, tensile strain can be achieved in the Ge-on-Si.^{24,25} The tensile strain up to 3.1%

TABLE I. The band parameters at 300 K for bulk Ge and Si (Ref. 9).

Parameter	Ge	Si
a (Å)	5.6573	5.4307
m_c (m_0)	0.038	0.528
m_{lL} (m_0)	1.57	1.659
m_{tL} (m_0)	0.0807	0.133
γ_1	13.38	4.22
γ_2	4.24	0.39
γ_3	5.69	1.44
E_p (eV)	26.3	21.6
E_g^Γ (eV)	0.7985	4.185
E_g^L (eV)	0.664	1.65
Δ (eV)	0.29	0.044
a_c (eV)	-8.24 ^a	1.98
a_v (eV)	1.24 ^a	2.46
a_L (eV)	-1.54 ^b	-0.66
b (eV)	-2.9	-2.1
C_{11} (10 GPa)	12.853	16.577
C_{12} (10 GPa)	4.826	6.393
n_r	4.02	3.4

^aReference 23.

^bReference 14.

FIG. 1. Band lineups of the Ge/Ge_{0.986}Si_{0.014} QW under different tensile strains in Ge layer. The GeSi layer is unstrained.

FIG. 2. Electron and hole energy dispersion curves of the Ge/Ge_{0.986}Si_{0.014} QW under different strains.

is reported in Ref. 25. The tensile strain shifts down both Γ and L conduction band edges, but the Γ band edge decreases faster than the L band edge due to the larger deformation potential at Γ point. At the strain of 1.61%, the band edges of Γ and L merge together, see Fig. 1, which is in agreement with the 1.9% calculated by the 30 band $k \cdot p$ method in Ref. 11. When the strain is larger than 1.61%, Ge becomes direct-bandgap. Under the tensile strain, the valence band maximum (VBM) becomes light hole band. The smaller effective mass of light hole will enhance the optical transition matrix elements. Fig. 2 shows the electron and hole energy dispersion curves of the Ge/Ge_{0.986}Si_{0.014} QW under the three different strains. When increasing the tensile strain

up to 2%, the second valence subband becomes light hole band as well as the top of valence subband. The weak anisotropy of valence subband energy dispersion curves is observed in the tensile strained Ge/GeSi QWs because the difference of γ_2 and γ_3 Luttinger parameters of Ge is very small, see Table I.

Energy dispersion curves (a) and equal-energy contour plots of the first subband (b) of electrons at L valley of the Ge/Ge_{0.986}Si_{0.014} QW are shown in Fig. 3. The contour plot energy range is from 600 to 2600 meV in step of 200 meV. The band bending is found along [110] direction due to the anisotropy effective mass of electron in L valley, which may result in negative value of the second term in Eq. (1). When

FIG. 3. Energy dispersion curves (a) and equal-energy contour plots of the first subband (b) of electrons at L valley of the Ge/Ge_{0.986}Si_{0.014} QW. The contour plot energy range is from 600 to 2600 meV in step of 200 meV.

FIG. 4. Γ and L valley electron concentrations versus their total electron concentrations for the Ge/Ge_{0.986}Si_{0.014} QW.

increasing the tensile strain, the band bending is weakened, see the first electron subbands in Fig. 3.

Fig. 4 shows the Γ and L valleys' electron concentrations versus their total electron concentrations for the Ge/Ge_{0.986}Si_{0.014} QW. Because the Γ and L conduction band edges are very close and the density of states of L subbands is very large, the leakage of electrons into L valley is significant. So, most electrons will occupy the L subbands, only a few percentage of electrons will occupy the Γ subbands. When increasing the tensile strain, more and more electrons will move into the Γ valley. The reason is that the tensile strain shifts down the Γ subbands faster than the L subbands. For total electron concentrations of $38 \times 10^{18} \text{ cm}^{-3}$, the ratio for electron to occupy L subbands, n_L/n_{total} is 0.023%,

0.82%, and 1.56% for the strain of 0.13%, 1.61%, and 2%, respectively.

Now we investigate the tensile strain influence on the optical gain of the Ge/Ge_{0.986}Si_{0.014} QWs. Fig. 5 shows the TM mode optical gain (a) and spontaneous radiative recombination rate spectra (b) of the 112/85 Å Ge QWs under the different tensile strains. The n-type doping concentration in the Ge well is $30 \times 10^{18} \text{ cm}^{-3}$. The injection carrier concentration is $8 \times 10^{18} \text{ cm}^{-3}$. For the tensile strain, the TM mode gain is greater than the TE mode gain, only the TM mode gain is shown here. When increasing the tensile strain, the gain will increase and the optical transition energy will decrease. When the strain is less than 1%, the gain is very weak. In order to achieve the significant gain, the tensile

FIG. 5. TM mode optical gain (a) spontaneous radiative recombination rate spectra (b) of the 112/85 Å Ge/Ge_{0.986}Si_{0.014} QW under different tensile strains. The n-type doping concentration in the Ge well is $30 \times 10^{18} \text{ cm}^{-3}$. The injection carrier concentration is $8 \times 10^{18} \text{ cm}^{-3}$.

FIG. 6. TM mode optical gain (a) spontaneous radiative recombination rate spectra (b) of the 112/85 Å Ge/Ge_{0.986}Si_{0.014} QW with the different n-type doping concentrations in the Ge well. The injection carrier concentration is $8 \times 10^{18} \text{ cm}^{-3}$. The tensile strain in the Ge QW is 1.61%.

strain needs to be greater than 1%. In Fig. 5(b), the tensile strain enhanced spontaneous radiative recombination rate spectra can be observed clearly. The calculated spontaneous radiative recombination rate spectrum with strain of 0.13% is in good agreement with the direct band-gap photoluminescence measurement in Ref. 22. The indirect band-gap transition is not taken into consideration in our simulation results.

Now, we study the n-type doping effect in the Ge QWs. Fig. 6 shows the TM mode optical gain (a) and spontaneous radiative recombination rate spectra (b) of the Ge/Ge_{0.986}Si_{0.014} QW with the different n-type doping concentrations in the well. The injection carrier concentration is $8 \times 10^{18} \text{ cm}^{-3}$. The tensile strain in the Ge QW is 1.61%. One can see that when the well is undoped, there is no optical gain. When increasing the n-type doping concentration in the well from $N_d = 10$ to $30 \times 10^{18} \text{ cm}^{-3}$, the peak optical will increase from 253 cm^{-1} up to 1508 cm^{-1} . In Fig. 6(b), the direct band gap spontaneous radiative recombination rate is very small for the undoped QW because a few electrons occupy the Γ conduction subbands. When the well is doped with n-type dopant, more and more electrons will be injected into the Γ valleys. For the $N_d = 10$ to $30 \times 10^{18} \text{ cm}^{-3}$, the peak spontaneous radiative recombination rate will be enhanced 22.5 to 51.3 times of the undoped QW case, respectively. Our results agree with the n-type doping enhanced photoluminescence measurement in Ge-on-Si reported recently.²⁶

Fig. 7 shows the TM mode gain spectra of the strained Ge QW at different injection carrier concentrations. The well doping concentration is $N_d = 30 \times 10^{18} \text{ cm}^{-3}$ and strain is 1.61%. The optical gain increases with the injection carrier concentration. The peak gain is up to 1936 cm^{-1} at injection carrier concentration of $10 \times 10^{18} \text{ cm}^{-3}$. The curves of peak gain versus injection carrier concentrations are plotted in Fig. 8. TM mode peak gain is greater than TE mode peak gain due to the tensile strain. Because the free carrier absorption cannot be ignored at very high carrier concentration, the curve of free carrier absorption loss versus injection carrier concentration is given in Fig. 8. The FCA loss is greater than the TE mode peak gain; pure TM mode polarized optical gain can be obtained. The inset shows the net TM mode peak gain versus inject carrier concentration. The transparent

FIG. 7. TM mode gain spectra of the strained Ge QW at different injection carrier concentrations. The well doping concentration is $N_d = 30 \times 10^{18} \text{ cm}^{-3}$.

FIG. 8. Curves of peak gain and free carrier absorption loss versus injection carrier density. The n-type doping concentration in Ge is $30 \times 10^{18} \text{ cm}^{-3}$. The inset shows the net peak gain versus inject carrier density.

injection carrier density is around $4 \times 10^{18} \text{ cm}^{-3}$. The net TM mode peak gain can be achieved up to about 1153 cm^{-1} at injection carrier concentration of $10 \times 10^{18} \text{ cm}^{-3}$. Note that it is a big challenge to produce such larger strain and doping level in the Ge/GeSi QW. Recently, a novel method was reported to introduce sustainable biaxial tensile strain larger than 1%²⁷ and 1.78%²⁸ in a thin Ge membrane using an integrated stressor layer. On the other hand, a delta-doping technique during epitaxial growth of Ge can achieve n-type doping level up to $4 \times 10^{19} \text{ cm}^{-3}$ in Ref. 6.

IV. CONCLUSIONS

Tensile-strain and doping enhanced direct bandgap optical transition of the n^+ doped Ge/GeSi quantum wells has been investigated by the multiple-band k-p method systematically. When tensile strain is greater or equal to 1.61%, Ge will become a direct band gap semiconductor and the Ge/Ge_{0.986}Si_{0.014} QW is type I. Introducing tensile strain and n-type dopant in the Ge QW can push more electrons into the Γ valleys and the direct bandgap optical gain can be achieved. The free carrier absorption loss can be greater than the TE mode peak gain; the pure TM mode polarized optical gain up to 1153 cm^{-1} can be obtained.

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