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Study of Nano-Scale Si/SiGe Structures for Quantum Cascade Emitters

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Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research and has not been submitted for a higher degree to any other University or Institution.

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Table of Contents

Acknowledgement.....i
Table of Contentsii
Summary..... iii
List of Figures.....iv
List of Tables.....v
Chapter 1 Literature Review1
 1.1 Scope..... 1
 1.2 Objectives 1
 1.3 Introduction..... 1
 1.3.1 Potential Applications3
 1.3.2 Motivation.....4
 1.3.3 Challenges and Objectives.....5
 1.4 Report Overview7
Chapter 2 Theoretical Review.....8
 2.1 Quantum Well Physics8
 2.2 Strain Effect on SiGe/Si Heterostructure9
 2.3 Quantum Cascade Structure..... 12
 2.4 k·p Method21
Chapter 3 Design Methodology23
 3.1 Eight-band k·p Model23
 3.2 Parameters Used in Calculations26
Chapter 4 Results and Discussions.....29
 4.1 Single Quantum Well Interdiffusion (Thermal Stability) Analysis.....29
 4.2 Coupling Effect in Coupled Quantum Wells38
 4.3 Triple Quantum Well Structure with Electric Field47
Chapter 5 Conclusion and Recommendations52
 5.1 Conclusion52
 5.2 Recommendations for Future Work52
Bibliography54
Author’s Publications58

Summary

Silicon is the dominant semiconductor in the microelectronics industry. Over the last 40 years, it has gone through the most amazing technological transformation and growth, which leads to the extraordinary high levels of integrated circuit complexities. The desire to integrate optical and microelectronic functions on the same chip to realize optoelectronic integrated circuits (OEICs) based on silicon ideally requires the active photonic components to be integrated with the silicon-based platform. Silicon-Germanium (SiGe) compound used as optoelectronic emission material attracts more and more attention due to the development of quantum cascade laser (QCL). Many researchers proposed different designs to realize the emission. However, it is yet successful. In this report, we analyzed the mechanisms in QCLs, and calculated the band structure with eight-band $k \cdot p$ method, with strain effect taken into consideration. Based on our calculations, we optimized the design to achieve an emission wavelength in far-infrared region.

List of Figures

Figure 2.1	(a) Schematic diagrams of a thin $\text{Si}_{1-x}\text{Ge}_x$ film and a thin $\text{Si}_{1-y}\text{Ge}_y$ film ($y < x$). (b) Schematic diagram of the two films in (a) placed together with the top film under compressive strain. (c) Schematic diagrams of a thin $\text{Si}_{1-y}\text{Ge}_y$ film and a thin $\text{Si}_{1-x}\text{Ge}_x$ film ($y < x$). (d) Schematic diagram of the two films in (c) placed together with the top film under tensile strain... 10
Figure 2.2	Schematic diagram of the conduction band of quantum cascade laser... 13
Figure 2.3	Schematic diagram of the band structure and intersubband transitions in the active region of the quantum cascade structure in Figure 2.2..... 13
Figure 2.4	Schematic diagram of the quantum staircase structure..... 15
Figure 2.5	E-k diagram of an inverted or negative effective mass structure..... 17
Figure 2.6	Schematic diagram of the quantum staircase structure based on HH2 to LH1 optical transitions..... 18
Figure 2.7	Schematic diagram of the quantum staircase structure based on interwell or diagonal transitions..... 19
Figure 2.8	Schematic diagram of mini-band cascade structure..... 20
Figure 3.1	Band edges of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ quantum well under compressive strain..... 28
Figure 4.1	Schematic diagram and TEM scan of 10-period MQWs..... 30
Figure 4.2	Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for sample (from top to bottom) 31
Figure 4.3	Cross sectional TEM micrographs of sample 32
Figure 4.4	Measured PL spectra of SiGe/Si single quantum well at different RTA temperature 33
Figure 4.5	Dependence of electron, heavy hole and light hole confinement potentials on diffusion lengths 34
Figure 4.6	Dependence of (a) C1-HH1 transition energy and (b) calculated PL-peak shift for $\text{Si}_{0.65}\text{Ge}_{0.35}/\text{Si}$ QW on diffusion length..... 36
Figure 4.7	Estimated diffusion coefficient D as a function of inverse temperature and activation energy for $\text{Si}_{0.65}\text{Ge}_{0.35}/\text{Si}$ QW..... 37
Figure 4.8	Schematic of coupled quantum wells 38
Figure 4.9	Comparison between band structures of $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ coupled quantum wells and single quantum well..... 39
Figure 4.10	Comparison of wave functions between $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ CQW and SQW.. 41
Figure 4.11	Energy dependence as a function of barrier width in $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ CQW. The two well widths are 50 and 100Å. 42
Figure 4.12	Energy dependence as a function of well width L_{z1} 43
Figure 4.13	Energy dependence as a function of Ge composition in well material. .. 44
Figure 4.14	PL spectra of samples D6 and M3..... 45
Figure 4.15	PL spectra of samples D1, D2, D3, D4, D5 and M2. 46
Figure 4.16	Energy states in designed structure with applied electric field 50

List of Tables

Table 3.1 Band parameters used in calculations.....27

Table 4.1 Electron and hole components in different energy states40

Chapter 1 Literature Review

1.1 Scope

This report describes the work carried out during my Master of Engineering (M.Eng) study and research. Essentially the report presents the research work done on Si/SiGe quantum cascade emitters (QCEs). Theoretical methods to design the emitter are described and the result of calculation is compared with experimental result and existing literature. The results obtained recently and plans for future work are included in this report.

1.2 Objectives

- a) Study the interdiffusion effect of Si-Ge (thermal stability) in Si/SiGe single quantum well.
- b) Investigate the coupling effect in adjacent wells with thin barrier.
- c) Calculate the band structures of three quantum wells systems, including coupling effect.

1.3 Introduction

In 1971, Rudolf Kazarinov and Robert Suris proposed that optical amplification could occur between the quantized electronic states of a multiple quantum-well structure under a high electric field [1]. In the late 1970s, scientists at Bell Laboratories began a 15-year research effort that concentrated on designing and growing artificially

structured semiconductor materials and devices of ever increasing complexity and functionality. This effort culminated in 1994 with the invention of the quantum cascade laser (QCL) [2].

Quantum cascade laser is a unipolar (or single type of carrier) laser. It relies on the intersubband emission with the upper laser state designed to have population inversion by engineering the lifetime using bandgap engineering and subband lifetime engineering. The structure of the quantum cascade laser consists of a series of quantum wells and barriers which together make up both active regions and injector regions. Usually the active regions comprise the layers in which the radiative transitions occur among the subbands of quantum wells, while the injector regions comprise a series of interacting quantum wells. Since the quantum cascade laser only involves intersubband transitions, the emission wavelength is adjustable to cover the mid- to far-infrared (also called terahertz) region by bandgap engineering. It also provides a promising approach to realize lasing from indirect bandgap materials, such as silicon.

As is well known, silicon is the dominant semiconductor in microelectronics. It would be highly desirable to realize silicon based light emitters for integrating optical and microelectronic components on the same chip. Although the indirect bandgap nature of silicon prohibits the efficient radiative recombination of electrons and holes that results in optical emissions, the quantum cascade (QC) system provides a potential mechanism for lasing from Si. Recently, intersubband photoluminescence (PL) and

electroluminescence (EL) have been demonstrated in SiGe/Si QC structures [3-8]. We believe that the quantum cascade laser can be realized in the IV-IV hetero-system.

1.3.1 Potential Applications

Quantum cascade laser has attracted a great amount of attention since it was invented. The reason that the QCL becomes such a hot topic is that its emission wavelength is in the mid- to far-infrared region. The quantum cascade laser is the only solid-state laser that can access such a long wavelength region.

At present, the mid- to far-infrared region of the electromagnetic spectrum is underutilized. The reason is that it is difficult to realize cheap practical sources and detectors. However, there are a number of potential applications. Firstly, chemical spectroscopy and pollution monitoring can employ terahertz laser. There are many chemical species that have very strong characteristic rotational and vibrational absorption lines [9]. When light of the proper energy is absorbed, the molecule of the chemical species undergoes a transition from one mode to another [9]. Hence, by knowing the absorbed energy, the type of the chemical species can be determined. This kind of spectroscopies was originally performed with incoherent thermal sources of IR radiation and Fourier-transform spectrometers using cryogenic bolometric detection. Due to low power emitted per wavelength and low sensitivity of the detector, these systems are not capable of detecting small concentrations of chemicals

[10]. Therefore for the applications in chemical spectroscopy and pollution monitoring, the terahertz lasers is a very good practical choice.

Imaging employing terahertz was developed in the mid 1990s at Bell Laboratories [11, 12]. It is well known as “T-ray” imaging. In a “T-ray” imaging system, most imaging is performed using ultra-short terahertz pulses generated by femtosecond optical pulses incident on a photoconductor or non-linear crystal. Comparing with typical bolometric detection, this system is more sensitive, and it does not require any kind of cooling or shielding [13]. The “T-ray” imaging system is very useful for biomedical imaging. The demonstrations of skin cancer detection and normal biological tissue imaging have been reported recently [14-16].

Other applications include free space communication, which takes advantage of the low absorption atmospheric windows from 3-5 and 8-14 μm . Detection of biological weapon, monitoring manufacturing defects in automotive dashboards and fat content in package meats, even countermeasure systems to protect aircraft from missile attack are all cited as potential applications of terahertz lasers.

1.3.2 Motivation

Since the III–V terahertz quantum cascade laser was demonstrated, investigation of Si-based laser starts attracting much attention. This is because the SiGe/Si materials

system may have a number of physical advantages over the III-V compound semiconductors at the mid- to far-infrared wavelength range. Firstly, the thermal conductivity of the Si substrates is approximately three times greater than that of the III-V substrates, thus it is easier for Si substrates to dissipate excess heat. Secondly, there is negligible polar optical phonon scattering in the SiGe/Si materials system. The absence of this scattering mechanism potentially allows high-temperature operation and significantly enhances the intersubband lifetimes. This has been experimentally verified [17]. Other advantages include low cost, mature silicon processing techniques and the ability to integrate silicon-based optoelectronics with silicon microelectronics.

Furthermore, the QCL based on the p-type SiGe/Si heterostructures gives the possibility of realizing a true surface-emitting device without the aid of any grating. This is because the transitions in the valence band between the light hole (LH) and heavy hole (HH) subbands can also couple to the in-plane electric field dipoles (TE polarization), which result in surface-normal propagating radiation [18].

1.3.3 Challenges and Objectives

Although the SiGe/Si QCL has many potential applications, there are several major challenges that have to be faced. First, there is a large built-in strain caused by the lattice mismatch (up to 4.2%) between Si and SiGe alloy. By growing strain balanced

SiGe/Si superlattice structures on a relaxed SiGe buffer (also called virtual substrate), the large built-in strain may be accommodated. However, precise control for growing very thin strained layers is highly desired. Second, since the conduction band offsets of the SiGe/Si materials system are quite small, the valence band is usually used to make the SiGe/Si QCL. However, the band structure of the valence band is more complex than that of the conduction band. Next, the band offsets of the SiGe/Si materials system are generally smaller than those of the III-V compound semiconductor. The interfaces in the SiGe/Si materials system are normally less perfect than that in the III-V heterostructures, such as InGaAs/InAlAs. It is also difficult to obtain structures that provide low loss optical cavities in the SiGe/Si materials system.

Due to the above challenges, SiGe/Si quantum cascade lasers are not present till now. So a large research space is left for exploration, and recently quantum cascade emission devices have been demonstrated by several research groups. All of these research groups are using molecular beam epitaxy (MBE) system to grow their devices. However, in this project, an ultra high vacuum chemical vapor deposition (UHV-CVD) epitaxial system will be employed, and the QC structures will be grown on both Si and SiGe virtual substrates. The main objective of this project is to study the property of the SiGe/Si quantum cascade structure in the purpose of demonstrating emission devices based on the SiGe/Si materials system.

1.4 Report Overview

The chapters of this report are arranged in the following ways:

- Chapter 1: Literature Review
- Chapter 2: Theoretical Review
- Chapter 3: Design Methodology
- Chapter 4: Results and Discussions
- Chapter 5: Summary and Future Plans

Chapter 1 includes a scope overview and my objectives on the project, and then starts with a brief introduction of the development on QCLs.

Chapter 2 gives a brief introduction on the theory of QCLs, which includes the basic quantum well physics and mechanism of QCL structure.

Chapter 3 describes the methods and parameters being used in the calculations

Chapter 4 presents results and discussions from different heterostructures: Single well, double wells and three wells system. Some experimental results are also derived to compare with theoretical results.

Chapter 5 draws the conclusion and recommendations.

Chapter 2 Theoretical Review

2.1 Quantum Well Physics

In 1926, Erwin Schrödinger developed a general theory of quantum mechanics. This theory is referred to as wave mechanics, it has been verified in many different experimental investigations, and has turned out to be the simplest and most useful general approach to quantum physics. The laws of conservation of energy, momentum, and angular momentum are held as basis assumption of quantum physics.

A typical quantum well (QW) is made of alternate layers of two different semiconductor materials. Since there is a difference in the conduction band alignment in these material layers, a series of potential barriers is formed analogous to the quantum barriers. The simplification of effective mass theory can be brought about using envelope function approximation, in which the electrons can be treated as plane waves in free space. The effects of the atomic potentials are accommodated by substituting the mass of a free electron by the effective mass m^* of the material.

Schrödinger equation (2.1) is the most popular one and it usually gives satisfactory description to the energy levels in quantum wells [6]

$$\left[-\frac{\hbar^2}{2m^*} \nabla^2 + V_{(z)} \right] \psi_{(z)} = E \psi_{(z)} \quad (2.1)$$

where $m^* = m_{well}$ in the well and $m^* = m_b$ in the barrier region.

In the presence of the quantum well potential,

$$V_{(z)} = \begin{cases} V_0 & |z| > \frac{L_w}{2} \\ 0 & |z| \leq \frac{L_w}{2} \end{cases} \quad (2.2)$$

where all energies are measured from the conduction band edge.

The eigenvalue and the eigenfunction can be obtained from the equation (2.1). Here we ignore the $k_{||} (k_{||}^2 = k_x^2 + k_y^2)$ dependence of $\psi_{(z)}$. Equation (2.1) is usually solved at $k_{||} = 0$ for the n th subband energy $E_n(0)$ with a wave function $\psi_{(z)} = f_n(z)$. On the other hand, in the direction along x-y plane, the electron moves as free particles and the energy can be described as

$$E_{(k)} = \frac{\hbar^2 k^2}{2m^*} \quad (2.3)$$

Then we have

$$E_n(k_{||}) = E_n(0) + \frac{\hbar^2 k_{||}^2}{2m_w} \quad (2.4)$$

2.2 Strain Effect on SiGe/Si Heterostructure

Since there is 4.2% lattice mismatch between Si and Ge (the lattice constants of Si and Ge are 5.43Å and 5.65Å, respectively), strain exists in the SiGe/Si materials system. Figure 2.1 gives a visual explanation on how compressive and tensile strains are formed in the SiGe/Si materials system. If a thin $\text{Si}_{1-x}\text{Ge}_x$ film is grown on bulk Si or $\text{Si}_{1-y}\text{Ge}_y$ ($y < x$) virtual substrate (a thick relaxed SiGe layer grown on Si substrate through grading layers), the film receives a biaxial compressive strain. If a thin Si or

$\text{Si}_{1-x}\text{Ge}_x$ film is grown on a $\text{Si}_{1-y}\text{Ge}_y$ ($y > x$) virtual substrate, the film receives a biaxial tensile strain. In both cases, the strains are formed in the plane that is perpendicular to the growth direction. The strains are in two directions within the plane, so the term biaxial is used.

Figure 2.1 (a) Schematic diagrams of a thin $\text{Si}_{1-x}\text{Ge}_x$ film and a thin $\text{Si}_{1-y}\text{Ge}_y$ film ($y < x$). (b) Schematic diagram of the two films in (a) placed together with the top film under compressive strain. (c) Schematic diagrams of a thin $\text{Si}_{1-y}\text{Ge}_y$ film and a thin $\text{Si}_{1-x}\text{Ge}_x$ film ($y < x$). (d) Schematic diagram of the two films in (c) placed together with the top film under tensile strain. [19]

As shown in Figure 2.1, the unstrained lattice parameters of the two layers are defined as a_A and a_B , respectively, while h_A and h_B are defined as the thickness of the respective layer. In Figure 2.1(b), the lattice constants of the two layers in the

interface plane are supposed to be the same. They are defined as $a_{//}$, while $a_{A\perp}$ and $a_{B\perp}$ are defined as the lattice constants of the two layers in the growth direction. Here, A and B represents the $\text{Si}_{1-x}\text{Ge}_x$ and $\text{Si}_{1-y}\text{Ge}_y$, respectively. In this materials system, $a_{//}$, $a_{A\perp}$ and $a_{B\perp}$ can be expressed by the following equations [20]:

$$a_{//} = (a_A G_A h_A + a_B G_B h_B) / (G_A h_A + G_B h_B) \quad (2.5)$$

$$a_{A\perp} = a_A [1 - D_A (a_{//} / a_A - 1)] \quad (2.6a)$$

$$a_{B\perp} = a_B [1 - D_B (a_{//} / a_B - 1)] \quad (2.6b)$$

In equation (2.5), $G_{A,B}$ is the shear modulus of each layer. When h_A is much larger than h_B , i.e. a thin $\text{Si}_{1-x}\text{Ge}_x$ film is grown on a Si substrate or $\text{Si}_{1-y}\text{Ge}_y$ virtual substrate, equation (2.5) can be reduced to $a_{//} \cong a_A$. In equation (2.6), $D_{A,B}$ is a constant that depends on the elastic constants c_{11} , c_{12} and c_{44} of the respective materials, and on the interface orientation. $G_{A,B}$ and $D_{A,B}$ are expressed as follows [20]:

$$G_{A,B} = 2(c_{11}^{A,B} + 2c_{12}^{A,B}) (1 - D_{A,B} / 2) \quad (2.7)$$

$$D_{001} = 2(c_{12}/c_{11}) \quad (2.8a)$$

$$D_{110} = (c_{11} + 3c_{12} - 2c_{44}) / (c_{11} + c_{12} + 2c_{44}) \quad (2.8b)$$

$$D_{111} = 2(c_{11} + 2c_{12} - 2c_{44}) / (c_{11} + 2c_{12} + 4c_{44}) \quad (2.8c)$$

It should be noted that only for (001) orientation, the value given for $a_{//}$ corresponds to the actual lattice constant in the crystallographic plane of the interface. $a_{//}$ and $a_{A,B\perp}$ express how the dimensions of the appropriate unit cell change with respect to the unstrained bulk unit cell [20].

According to Vegard's law, the lattice constant of a $\text{Si}_{1-x}\text{Ge}_x$ alloy layer can be predicted with accuracy to about 10^{-4} nm [21]:

$$a_{\text{Si}_{1-x}\text{Ge}_x} = 0.5431 + 0.01992x + 0.0002733x^2 \text{ (nm)} \quad (2.9)$$

Elastic constants c_{11} and c_{12} of the SiGe alloy can be determined by the linear interpolation approach. Hence, the strain components parallel and perpendicular to the interface could be easily obtained [20]:

$$\varepsilon_{A,B//} = (a_{//}/a_{A,B} - 1) \quad (2.10)$$

$$\varepsilon_{A,B\perp} = (a_{A,B\perp}/a_{A,B} - 1) \quad (2.11)$$

By combining equations (2.5) and (2.10), the relation between $\varepsilon_{A//}$ and $\varepsilon_{B//}$ can be expressed by the following equation:

$$\varepsilon_{A//} = -\left(\frac{G_B h_B}{G_A h_A}\right) \varepsilon_{B//} \quad (2.12)$$

Theoretically speaking, a superlattice structure consisting of infinite layers of strain balanced $\text{Si}_{1-x}\text{Ge}_x$ and Si films can be grown.

2.3 Quantum Cascade Structure

As stated in Chapter 1, the QCL is unipolar laser, which is based on intersubband transitions in quantum wells [2]. For III-V semiconductor, electron transitions in the conduction band are usually used to develop the QCL, while the SiGe/Si QCEs use hole transitions in the valence band. This is because most of band offset occurs in the

valence band for pseudomorphic growth on Si substrates. For pseudomorphic growth on a relaxed SiGe buffer, the band offset obtained in the conduction band are still not as large as those available in the valence band.

Figure 2.2 Schematic diagram of the conduction band of quantum cascade laser [21]

Figure 2.3 Schematic diagram of the band structure and intersubband transitions in the active region of the quantum cascade structure in Figure 2.2 [22].

There are several different designs for achieving population inversion in the active quantum cascade elements [18, 19]. A typical band structure of QCL is illustrated in Figure 2.2. This structure comprises two parts: the active and injector region. The injector region is formed by a chirped superlattice structure, where the mini-band is formed. The active region can be illustrated in Figure 2.3. It is a four level system (it is also considered as a three level system in some literature, because energy level E_1 is E_4 in the adjacent downstream active region). The carriers coming from energy level E_4 tunnel across the barrier into energy level E_3 of the quantum well. Due to the existence of a forbidden energy mini-band resulting by the chirped superlattice collector, the carriers cannot easily tunnel into continuum states and have to recombine in the quantum wells. Therefore, the carriers will transit to the energy level E_2 , then to energy level E_1 . In order to achieve the population inversion in the active region, the lifetime for transition from E_2 to E_1 must be significantly less than the lifetime for transition from E_3 to E_2 . This could be realized by designing the energy separation of energy level E_2 and E_1 to be resonant with the optical phonon energy in the host material. At the same time, the transition from E_3 to E_2 must involve significant momentum transfer in terms of optical phonon emission, so that the lifetime for transition from E_3 to E_2 becomes as long as possible. The barriers and quantum wells must be of the appropriate composition and thickness so that under the influence of an electric field, the energy level E_1 becomes resonant with the energy level E_3 in the adjacent downstream active region. Hence, under the influence of the electric field, the carriers will release photons in each active region. If the optical

feedback is made available, the laser oscillation over these transitions becomes possible. However, this structure requires a highly accurate growth control. Any error of the quantum well thickness or composition may reduce the efficiency of the laser or even destroy the whole cascade structure.

Figure 2.4 Schematic diagram of the quantum staircase structure [23]

A second design (as shown in Figure 2.4) was firstly proposed by Friedman *et al.* [23, 24]. It is relatively simpler than the previous one. The structure comprises injector, active region and collector. The active region is formed by a superlattice structure. In this structure, the radiative transitions occur within each quantum well and the carriers transit from well to well by non-radiative transitions from first heavy hole subband (HH1) to first light hole subband (LH1). The HH1 energy level could become resonant

with the LH1 energy level in the adjacent downstream quantum well under the influence of an electric field. The electric field F could be estimated by the following equation [23]:

$$F = E_{\text{LH-HH}} / (w + b) \quad (2.13)$$

where $E_{\text{LH-HH}}$ is the energy separation between the LH and HH states, w and b are the thickness of the QWs and barriers respectively.

In order to attain population inversion in the quantum staircase structure, the total interwell transition rate (from HH1 to LH1) must be faster than the total intrawell transition rate (from LH1 to HH1). However, the interwell transition rates in QCLs are generally dominated by the incoherent scattering processes, rather than coherent tunneling. In p-type SiGe/Si materials system, the effective masses of the carriers (holes) in the Si barriers are much larger than those in the n-type III-V materials system. Hence, the tunneling rate of these carriers will be even slow. Therefore, it is rather difficult to attain population inversion in this system. Obviously, reducing the barrier widths helps to increase the tunneling rate (from HH1 to LH1). However, the improvements are quite limited by the available growth technique.

One possible way of improving the basic quantum staircase design is by utilizing the inverted or negative effective mass feature [23, 25], as shown in Figure 2.5. This could be achieved by engineering the LH1 subband. Since the selection rules forbid the LH1 and HH2 subbands to cross, by bending the LH1 subband upwards to a

higher hole energy will result in an anticrossing with the HH2 subband. Hence, the LH1 subband is forced to have a negative effective mass structure. An LH1 to HH1 subband pair then form the basis of a four level unipolar laser, as shown in Figure 2.5. The holes are injected from the adjacent upstream quantum well at the zone center ($k=0$), and then relax to the LH1 subband minimum, which is at a finite k . Thereafter, these holes transit to the HH1 subband with photon emission. Finally, these holes relax towards the zone center of HH1 subband, and then transit to the adjacent downstream quantum well. The advantage of the negative effective mass structure is that population inversion (in k -space) is readily attained due to the favorable band curvature of LH1 and HH1 respectively. Unfortunately, the negative effective mass structure in SiGe/Si materials system is weak and can easily be removed by applying a small electric field. An accurate growth control of this structure is also highly desired. Any error in the control of quantum well thickness and composition can shift the subbands and destroy the negative effective mass feature.

Figure 2.5 E-k diagram of an inverted or negative effective mass structure [18]

Another way to improve the basic quantum staircase structure is by involving the HH2 to LH1 transitions [18], as shown in Figure 2.6. In this structure, each quantum well contains three active subbands: the HH2, LH1 and HH1 subbands. Under the influence of an electric field, we could attain near-resonance between HH1 and the HH2 subband in the downstream well. The holes transit from HH2 to LH1 with photon emission, and then depopulate to HH1 by non-radiative LH1 to HH1 scattering. Thereafter, these holes tunnel from HH1 to the HH2 subband in the downstream quantum well. Comparing with the basic quantum staircase structure, the optical transition from HH2 to LH1 is fully allowed at the zone center, and the interwell coupling of HH1 and the HH2 subbands in the downstream quantum well is much strong. However, in the steady state, a substantial percentage of the carriers reside in the HH1 subbands in each quantum well, which will cause a loss in quantum efficiency.

Figure 2.6 Schematic diagram of the quantum staircase structure based on HH2 to LH1 optical transitions [18].

The interwell or diagonal optical transition is another mean to improve the prospects of population inversion in the basic quantum staircase structure [5, 18]. In such a structure, the HH1 subband becomes the upper laser level; while the LH1 subband in the downstream quantum well is the lower laser level, as shown in Figure 2.7. In this design, obtaining population inversion is relatively easier, since the majority of carriers generally occupy the HH1 subbands. However, the device must be biased such that the HH1 and the downstream LH1 subbands are separated by the required photon energy at the zone center. In addition, a thinner barrier ($<2\text{nm}$) is required to obtain efficient optical transitions.

Figure 2.7 Schematic diagram of the quantum staircase structure based on interwell or diagonal transitions [18]

Besides the quantum staircase structure, optical transition between mini-band states is another approach to realize the QCLs [26]. In this structure, the transitions of carriers

take place between the mini-bands rather than the discrete subbands. Mini-band transitions allow higher currents to produce linewidth narrowing followed by lasing. However, the mini-band cascade structure requires chirped superlattice layers with very thin barriers. Each period contains up to 30 layers. The growth requirements of this structure are even higher than that of the structures given above.

Figure 2.8 Schematic diagram of mini-band cascade structure [19]

Among the various designs of the quantum cascade structures, the design shown in Figure 2.2 has been proved feasible in the III-V materials system [27]; furthermore, the intersubband electroluminescence from SiGe/Si materials system has been demonstrated using this design [28]. However, the growth of quantum staircase structure is relatively easier, and the structure with relatively low Ge fraction (<30%) has been proved feasible as well [29, 30].

2.4 $k \cdot p$ Method

For a period potential, the electronic band structure and the wave function can be derived from the Hamiltonian, which satisfied the symmetry of the semiconductor crystals. Numerical methods to find the band structures and the wave functions include the tight binding, the pseudopotential, the orthogonalized plane wave, the augmented plane wave, Green's function, and the cellular methods. Our interest here is near the band edges, where the wave vector k deviates by a small amount from a vector k_0 where a local minimum or maximum occurs. Starting from the Schrödinger's equation

$$\left[\frac{p^2}{2m} + V_{(r)} \right] \Psi_{n,k(r)} = E_{n,k} \Psi_{n,k(r)} \quad (2.14)$$

Replacing $\Psi_{n,k(r)}$ by $u_{n,k(r)} \exp(ik \cdot r)$ we can get that

$$\left[\frac{p^2}{2m} + \frac{\hbar k \cdot p}{m} + \frac{\hbar^2 k^2}{2m} + V_{(r)} \right] u_{n,k(r)} = E_{n,k} u_{n,k(r)} \quad (2.15)$$

we assume that we know the value of $E_{n,0}$ either from experiment or theory. We then consider small values of k close to $k = 0$ and treat the operator $\frac{\hbar}{m} k \cdot p$ as a perturbation in the Hamiltonian.

The $k \cdot p$ method is a semi-empirical method which uses quantities found from experiments in the theoretical calculation of the band structures and has been applied by many researchers to semiconductors and very popular in studying bulk and quantum well semiconductors. It is much easier to apply for analyzing the band structure near a particular point k_0 , especially when it is near an extreme of the band

structure. Here we consider that the extreme occurs at the zone center where $k_0=0$.

In this chapter, we have reviewed the quantum well physics, strain effect on the band structure of SiGe/Si heterostructures. The history of QCLs was also reviewed. At the last section, we introduced the $k \cdot p$ method. Basically, like all kinds of optoelectronic devices, the fundamental of QCL is quantum mechanics and the performance strictly depends on the material growth technology. Layer crystalline property like strain also has significant effect on the band structure. In the next chapter, we will demonstrate how we applied the convenient $k \cdot p$ method in analyzing the material properties and design methodology.

Chapter 3 Design Methodology

3.1 Eight-band k·p Model

The Hamiltonian used to calculate the band structure, which includes the conduction, light-hole, heavy-hole, and spin-orbit split-off band, is consisted of three parts.

One is the non-strain part H_k , another is strain matrix H_s and the third is $V_{(z)}$, which is a scalar. Thus the whole Hamiltonian to be solved is

$$H = H_k + H_s + V_{(z)} \quad (3.1)$$

The Bloch wave function are given below,

$$|+\rangle = |S \uparrow\rangle$$

$$|-\rangle = |S \downarrow\rangle$$

$$\left|\frac{3}{2}\right\rangle = \left|i \left[-\frac{1}{\sqrt{2}} (X + iY) \uparrow \right] \right\rangle$$

$$\left|\frac{1}{2}\right\rangle = \left|i \left[\sqrt{\frac{2}{3}} Z \uparrow - \frac{1}{\sqrt{6}} (X + iY) \downarrow \right] \right\rangle$$

$$\left|-\frac{1}{2}\right\rangle = \left|i \left[\frac{1}{\sqrt{6}} (X - iY) \uparrow + \sqrt{\frac{2}{3}} Z \downarrow \right] \right\rangle$$

$$\left|-\frac{3}{2}\right\rangle = \left|i \left[\frac{1}{\sqrt{2}} (X - iY) \downarrow \right] \right\rangle$$

$$\left|\frac{7}{2}\right\rangle = \left|i \left[\frac{1}{\sqrt{3}} Z \uparrow + \frac{1}{\sqrt{3}} (X + iY) \downarrow \right] \right\rangle$$

$$\left|-\frac{7}{2}\right\rangle = \left|i \left[\frac{1}{\sqrt{3}} (X - iY) \uparrow - \frac{1}{\sqrt{3}} Z \downarrow \right] \right\rangle$$

Where S, X, Y, Z are the band-edge Bloch functions.

Taken in order of the basis functions, the 8x8 $k \cdot p$ Hamiltonian H_k is given by [31]

$$\begin{bmatrix} E_6^0 & 0 & \frac{-1}{\sqrt{2}}P^+ & \sqrt{\frac{2}{3}}P^z & \frac{1}{\sqrt{6}}P^- & 0 & \frac{1}{\sqrt{3}}P^z & \frac{1}{\sqrt{3}}P^- \\ 0 & E_6^0 & 0 & -\frac{1}{\sqrt{6}}P^+ & \sqrt{\frac{2}{3}}P^z & \frac{1}{\sqrt{2}}P^- & \frac{1}{\sqrt{3}}P^+ & \frac{-1}{\sqrt{3}}P^z \\ c.c. & 0 & E_8^{+0} & B & C & 0 & \frac{1}{\sqrt{2}}B & \sqrt{2}C \\ c.c. & c.c. & c.c. & E_8^{-0} & 0 & C & -\sqrt{2}U & -\sqrt{\frac{3}{2}}B \\ c.c. & c.c. & c.c. & 0 & E_8^{-0} & -B & -\sqrt{\frac{3}{2}}B^* & \sqrt{2}U \\ 0 & c.c. & 0 & c.c. & c.c. & E_8^{+0} & -\sqrt{2}C^* & \sqrt{\frac{1}{2}}B^* \\ c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & E_7^0 & 0 \\ c.c. & c.c. & c.c. & c.c. & c.c. & c.c. & 0 & E_7^0 \end{bmatrix}$$

where

$$k_{\pm} = k_x \pm ik_y$$

$$P^z = Pk_z$$

$$P^{\pm} = Pk_{\pm}$$

$$E_6^0 = E_g + \frac{\hbar^2}{2m_0} \tilde{k}^2$$

$$E_8^{+0} = -\tilde{\gamma}_1 \tilde{k}^2 + U$$

$$E_8^{-0} = -\tilde{\gamma}_1 \tilde{k}^2 - U$$

$$E_7^0 = -\Delta - \tilde{\gamma}_1 \tilde{k}^2$$

$$U = \tilde{\gamma}_2 \left(2\tilde{k}_z^2 - (\tilde{k}_x^2 + \tilde{k}_y^2) \right)$$

$$B = 2\sqrt{3}\tilde{\gamma}_3 \tilde{k}_z \tilde{k}_-$$

$$C = \sqrt{3} \left[\tilde{\gamma}_2 (\tilde{k}_x^2 - \tilde{k}_y^2) - 2i\tilde{\gamma}_3 \tilde{k}_x \tilde{k}_y \right]$$

$$\tilde{k}_j^2 = \frac{\hbar^2 k_j^2}{2m_0}, j = x, y, z$$

$$\tilde{\gamma}_1 = \gamma_1 - \frac{E_p}{3E_g}, \tilde{\gamma}_2 = \gamma_2 - \frac{E_p}{6E_g}, \tilde{\gamma}_3 = \gamma_3 - \frac{E_p}{6E_g}, \tilde{\gamma}_c = \frac{\hbar^2}{2m_0}$$

The momentum matrix element and the corresponding energy are

$$P = \langle S | P_x | iX \rangle \quad (3.2)$$

$$E_p = \frac{2m_0}{\hbar^2} P^2 \quad (3.3)$$

k is the wave vector, E_g is the energy gap of well material, m_0 is free electron mass,

$\gamma_1, \gamma_2, \gamma_3$ are the Luttinger parameters, which are normally used to express the

effective mass of valence band, and Δ is the spin-orbit split-off energy.

The H_s strain matrix is given by

$$\begin{bmatrix} 0 & 0 & \frac{1}{\sqrt{2}}\tilde{P}^+ & -\sqrt{\frac{2}{3}}\tilde{P}^z & -\frac{1}{\sqrt{6}}\tilde{P}^- & 0 & -\sqrt{\frac{1}{3}}\tilde{P}^z & -\sqrt{\frac{1}{3}}\tilde{P}^- \\ 0 & 0 & 0 & \frac{1}{\sqrt{6}}\tilde{P}^+ & -\sqrt{\frac{2}{3}}\tilde{P}^z & \frac{-1}{\sqrt{2}}\tilde{P}^- & -\sqrt{\frac{1}{3}}\tilde{P}^+ & \sqrt{\frac{1}{3}}\tilde{P}^z \\ c.c. & 0 & \varepsilon & 0 & 0 & 0 & 0 & 0 \\ c.c. & c.c. & 0 & -\varepsilon & 0 & 0 & -\sqrt{2}\varepsilon & 0 \\ c.c. & c.c. & 0 & 0 & -\varepsilon & 0 & 0 & \sqrt{2}\varepsilon \\ 0 & c.c. & 0 & 0 & 0 & \varepsilon & 0 & 0 \\ c.c. & c.c. & 0 & c.c. & 0 & 0 & 0 & 0 \\ c.c. & c.c. & 0 & 0 & c.c. & 0 & 0 & 0 \end{bmatrix}$$

Where

$$\tilde{P}^z = P e_{zz} k_z$$

$$\tilde{P}^\pm = P (e_{xx} k_x + i e_{yy} k_y)$$

$$\varepsilon = \frac{1}{2}b(e_{xx} + e_{yy} - 2e_{zz})$$

$$e_{xx} = e_{yy} = e_{//} = \frac{a_{\text{barrier}} - a_{\text{well}}}{a_{\text{well}}}$$

$$e_{zz} = e_{\perp} = -2\frac{C_{12}}{C_{11}}e_{//}$$

b is the valence-band shear strain deformation potential for the well, e_{xx} is the in-plane strain, C_{12} and C_{11} are elastic stiffness constants, and $V_{(z)}$ is the periodic potential of the quantum wells, is diagonal in the 8-dimension spinor basis, which is given by

$$V_{(z)} = \begin{cases} V_0(\Delta E_c) & \text{in barrier} \\ 0 & \text{in well} \end{cases} \quad (3.4)$$

3.2 Parameters Used in Calculations

In this chapter, various band parameters essential to the calculation of band structure and absorption are presented. The method used to calculate the band offset of quantum wells due to strain are given. Except for the unstrained indirect band gap energy, most parameters for $\text{Si}_{1-x}\text{Ge}_x$ are obtained by linear interpolation between the parameters of binary compound semiconductors as listed in Table 3.1, and is given by

$$P(\text{Si}_{1-x}\text{Ge}_x) = (1-x)P(\text{Si}) + xP(\text{Ge}) \quad (3.5)$$

	Si	Ge
Lattice constant a (Å)	5.431	5.658
Energy gap E_g (eV)	4.185	0.898
Spin-orbit splitting Δ (eV)	0.044	0.297
Kane energy E_p (eV)	21.6	26.3
Effective mass m_C (m_0)	0.528	0.038
Luttinger parameter γ_1	4.285	13.38
Luttinger parameter γ_2	0.339	4.24
Luttinger parameter γ_3	1.446	5.69
Deformation potential a_c (eV)	-5.1	-9.5
Deformation potential a_v (eV)	0	0
Shear deformation potential b (eV)	-2.1	-2.9
Stiffness C_{11} (GPa)	167.5	131.5
Stiffness C_{12} (GPa)	65.0	49.4

Table 3.1 Band parameters used in calculations (Ref. [32])

The unstrained indirect band gap energy of $\text{Si}_{1-x}\text{Ge}_x$ is given by [19]

$$E_g(\text{Si}_{1-x}\text{Ge}_x) = 1.155 - 0.43x + 0.0206x^2 \text{ eV} \quad (3.6)$$

The strain effect due to lattice mismatch can shift the band edge that we have to take into account during the calculations. For $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ QW it is mostly compressive strain. Now we discuss the compressive strain-induced band shift by looking at the Fig 3.1. The solid line represents the well structure before strain. The dotted line is the structure taking hydrostatic strain induced energy shift in both conduction and valence band into consideration. And the dashed line represents the energy shift due to shear strain induced shift in heavy hole and light hole.

Figure 3.1 Band edges of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ quantum well under compressive strain

For compressive strain, in-plane strain $\epsilon_{||}$ is negative and perpendicular strain $\epsilon_{\perp}$ is positive. The conduction band edge is shifted by [33]

$$\delta E_c = 2a_c \left(1 - \frac{C_{12}}{C_{11}} \right) \epsilon_{||} \quad (3.7)$$

The valence subbands are shifted by

$$\begin{aligned} \delta E_{hh} &= -P_{\epsilon} - Q_{\epsilon} \\ \delta E_{lh} &= -P_{\epsilon} + Q_{\epsilon} \end{aligned} \quad (3.8)$$

$$P_{\epsilon} = -2a_v \left(1 - \frac{C_{12}}{C_{11}} \right) \epsilon_{||} \quad Q_{\epsilon} = -b \left(1 + 2 \frac{C_{12}}{C_{11}} \right) \epsilon_{||}$$

The band edge after shifting is given by

$$E'_g(\text{Si}_{1-x}\text{Ge}_x) = E_g(\text{Si}_{1-x}\text{Ge}_x) + \delta E_c + P_{\epsilon} + Q_{\epsilon} \quad (3.9)$$

The band offset is chosen as $\Delta E_v = 0.84x$ for $\text{Si}_{1-x}\text{Ge}_x$.

Chapter 4 Results and Discussions

Our research process follows three steps, corresponding to study on single quantum well (SQW), double quantum well (DQW) and triple quantum well (TQW) respectively. SQW was used to study the thermal properties of SiGe structure, while DQW was used to study the coupling effect between adjacent wells in multi-well structure, and finally a TQW is to be designed to realize the quantum cascade emitter (QCE).

4.1 Single Quantum Well Interdiffusion (Thermal Stability) Analysis

As required by cascade structure, SiGe layers can be grown to very large thickness by symmetrically strained method, but thermal stability through nucleation dislocation and interdiffusion of Si-Ge atoms is still a critical issue especially when the high processing temperature is unavoidable. The interdiffusion of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ QWs has been reported in several literatures. However, different materials are used as well as the measuring methods, there exists a discrepancy in the literature on the value of thermal activation energy E_a in the range of 2eV~5eV. In our study, the E_a value is reexamined by applying the PL study on interdiffusion of SiGe/Si single quantum well undergoing a post-growth thermal treatment and the modified 6+2 band $k \cdot p$ method [34-36].

The samples were grown by the UHV-CVD system at 530°C (for the SiGe QW layers) and 600°C (for the Si barriers and capping layer). The higher growth temperature of the Si barriers and capping layer was chosen to enhance the growth rate of the relatively thick epilayers; hence the total process time could be shortened. The mixture of Si₂H₆ and GeH₄ were used as source gases to grow the SiGe epilayers on the (100) p-type Si substrates. In total, the sample was grown for 10 periods of Si_{0.65}Ge_{0.35} (L_z = 6nm)/Si (L_b = 40nm) layers and 10nm Si capping layers (as shown in Figure 4.1). These samples were characterized by the cross sectional TEM and high resolution XRD (HR-XRD).

Figure 4.1 Schematic diagram and TEM scan of 10-period MQWs

Postgrowth annealing was carried out in a N₂ gas flowing ambient for 100s. The annealing temperatures were ranged from 750°C to 900°C, and the increment is 50°C. The PL spectra was measured at 5K by standard lock-in techniques and detected with a liquid nitrogen cooled Ge detector. TEM scans were taken for both the as-grown and

900°C annealed samples.

Figure 4.2 Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for sample (from top to bottom)

High resolution XRD measurements were conducted to analyze the material quality and the compositions of sample. The sharp peaks with the highest intensity in the rocking curves arise from the Si substrate. The experimental rocking curves were compared with dynamical simulation to determine the physical parameters of the structures. As shown in Figure 4.2, the experimental XRD data of the samples are well reproduced by the dynamical simulation. However, compared with the simulated curves, certain satellite peaks are missing in the experimental results. This is due to the imperfect interfaces between the QWs and barriers, which could be observed in the cross sectional TEM micrographs of the samples (as shown in Fig 4.3).

Figure 4.3 Cross sectional TEM micrographs of the sample

The measured PL spectra of 6nm $\text{Si}_{0.65}\text{Ge}_{0.35}/\text{Si}$ quantum well structure are shown in Fig 4.4. The peaks corresponding to energies higher than 1 eV are silicon related. After annealing, the no-phonon (NP) transition and transverse-optic (TO) phonon assisted transition peaks are observed. Both of them are associated with SiGe layer. As the annealing temperature is increased, blueshifts of the NP peaks and increases of the PL intensity are also observed. The enhancement of the PL intensity is due to the reduction of the density of defects in the samples by annealing.

Figure 4.4 Measured PL spectra of SiGe/Si single quantum well at different RTA temperature

Following Ref. 37, we believe that the PL-peak shift is caused by Si-Ge atomic interdiffusion across the interface of the quantum well. The $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ disordered QW is modeled by setting x' as the composition of Ge atom after Si-Ge interdiffusion. The interdiffusion process is described by diffusion length L_d , which is equal to $(Dt)^{1/2}$, where t is the diffusion time and D is the diffusion coefficient. The Ge composition x' after diffusion is described as [34-36]

$$x'(z) = \frac{x}{2} \left[\text{erf} \left(\frac{L_z + 2z}{4L_d} \right) + \text{erf} \left(\frac{L_z - 2z}{4L_d} \right) \right], \quad (4.1)$$

where z is the length along growth direction, x is the as-grown composition of Ge, and L_z is the QW width before interdiffusion.

Figure 4.5 Dependence of electron, heavy hole and light hole confinement potentials on diffusion lengths: $L_d=0\text{nm}$ (solid line), $L_d=0.5\text{nm}$ (dashed line), $L_d=1\text{nm}$ (dotted line) and $L_d=1.5\text{nm}$ (dashed dotted line), with well center at $z=0$.

Fig 4.5 shows the dependence of electron (CB), heavy hole (HH), and light hole (LH) confinement profiles of the $6\text{nm Si}_{0.65}\text{Ge}_{0.35} / \text{Si}$ SQW structure along the grown axis with different diffusion lengths including the strain effect. The origin is taken to be the valence band maximum after strain. The valence band edge is actually the HH band edge due to compressive strain. The relationship between the HH and LH terms in the strained Hamiltonian matrix as

$$E_{lh}^s(x') = E_{hh}^s(x') + 2Q_\varepsilon(x'), \quad (4.2)$$

Where $Q_\varepsilon(x')$ is the shear strain energy term of $\text{Si}_{1-x}\text{Ge}_x$. Considering the interdiffusion effect, for the case of $L_d=1.5\text{nm}$, at the well center ($z=0\text{nm}$), E_{hh}^s and

$2Q_e$ are -40.7 and -97.3 meV, respectively, so that $E_{th}^s = -138$ meV. As z approaches the interface in the well region ($z=3.0$ nm), E_{hh}^s and $2Q_e$ are -130.1 and -58.6 meV, respectively, leading to $E_{th}^s = -188.7$ meV. It reveals that the increase of $2Q_e(x')$ (38.7 meV) is much slower than the reduction of $E_{hh}^s(x')$ (89.4 meV) in the well region. The similar observation applies to the case in the barrier region. The conduction band offset $\Delta E_c(x')$ is given by

$$\Delta E_c(x') = \Delta E_g(x') - \Delta E_v(x'), \quad (4.3)$$

Where $\Delta E_g(x')$ is the energy gap difference between the well and the barrier layer, and $\Delta E_v(x')$ represents the valence band offset. All the terms have been taken into account the influence of strain effect. As discussed, the alignment of the $\text{Si}_{0.65}\text{Ge}_{0.35}/\text{Si}$ QW is of type II, which means that $\Delta E_g(x')$ is less than $\Delta E_v(x')$. It give rises to a negative $\Delta E_c(x')$, i.e., the profile of CB, as shown in Fig 4.5.

Considering the interdiffusion effect, the dependence of transition energy (C1-HH1) on diffusion length was calculated by 6+2 band $k \cdot p$ method, as shown in Fig 4.6 (a). The calculated emission wave length of the as-grown sample is 1.342 μm (923.4 meV), which is close to the experimental NP transition peak 1.346 μm (921.2 meV). As L_d increases, a blueshift can be observed. Subsequently, the calculated transition energy shift ΔE as a function of L_d is shown in Fig 4.6(b).

Figure 4.6 Dependence of (a) C1-HH1 transition energy and (b) calculated PL-peak shift for Si_{0.65}Ge_{0.35}/Si QW on diffusion length.

The experimental data are fitted with the theoretically calculated ones. According to the equation of diffusion coefficient given by

$$D = D_0 \exp\left(-\frac{E_a}{KT}\right), \quad (4.4)$$

Where D is the diffusion coefficient and D_0 is a constant, we derive the activation energy E_a of 1.8 eV (see Fig 4.7), which is close to the literature referred 2.0 eV [37].

Figure 4.7 Estimated diffusion coefficient D as a function of inverse temperature and activation energy for $\text{Si}_{0.65}\text{Ge}_{0.35}/\text{Si}$ QW.

In short summary, the effect of annealing on the optical properties of $\text{Si}_{0.65}\text{Ge}_{0.35}/\text{Si}$ SQW structure is investigated by low temperature PL measurements. PL blueshift is observed and modeled by Si-Ge atomic interdiffusion in the study. The ground state transition energy of the as-grown sample calculated by 6+2 band $k \cdot p$ method of 923.4 meV agrees well with the measured 921.2 meV. As diffusion length increase, blueshift can be derived which agrees well with measurement. Finally, an E_a of 1.8 eV is obtained.

4.2 Coupling Effect in Coupled Quantum Wells

Among most quantum cascade structure designed, the active region contains more than one quantum well with thin barriers [2]. The wave functions are no longer confined to a single well but penetrate into barriers and extend over the whole region, which results in an interaction between energy states in nearby quantum wells called coupling. Therefore, part of my research work focus on the interwell coupling effect.

Firstly, to clarify the reliability of our method, the neighboring well width, L_{z2} is set to zero as shown in Fig 4.8(b). The structure becomes a SQW structure with barrier width L_b , well width L_{z1} and period $L = L_b + L_{z1}$.

Figure 4.8 Schematic of coupled quantum wells

When $k = 0$, measuring from the uppermost valence band edge of the well region, the

calculated energy levels of the SQW HH1= 45.3, HH2= 162.2, LH1= 89.3, LH2= 193.3 and SO1= 210.6 meV are in good agreement with ones reported by People *et al* [38], HH1= 43, HH2= 156, LH1= 91, LH2= 205, SO1= 192 meV, and ones reported by Kahan *et al* [39], HH1= 42, HH2= 155, LH1= 96, LH2= 199 and SO1= 215 meV, where SO1 is the first spin-orbit split off state energy. Fig 4.9 shows the comparison between the in-plane dispersion curves of the valence hole subbands confined in the coupled quantum well (CQW) and SQW.

Figure 4.9 Comparison between band structures of $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ coupled quantum wells and single quantum well. The solid line and dashed line show the band structure of QW L_{z1} with different barrier width $L_b = 20/60 \text{ \AA}$. While the dotted line shows the dispersion curves of $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ (50/200Å) SQW. The zero energy reference is taken as the average of the bottom energy levels of the heavy hole and light hole bands in the strained quantum well.

By comparison, the coupling effect in the CQW can be identified by the energy state changes, as well as the nonparabolic dispersions. Fig 4.10 shows the corresponding wave functions at $k=0$ as in Fig 4.9. Following Fig 4.8(a), the well widths are $L_{z1}=50\text{\AA}$ and $L_{z2}=100\text{\AA}$ respectively. The solid line and dashed line show the band structure of QW L_{z1} with different barrier width $L_b=20/60\text{\AA}$. The dispersion curves of $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ ($50/200\text{\AA}$) SQW are also plotted in dotted line. The used parameters are listed in Table 4.1. Energy states are identified by wave functions and the components of hh , lh and so [40, 41], as shown in Table 4.1.

Structure	Energy state	hh	lh	so
CQW $L_b=20\text{\AA}$	hh1	100%	0	0
	hh2	100%	0	0
	lh1+so1	0	94.5%	5.5%
CQW $L_b=60\text{\AA}$	hh1	100%	0	0
	hh2	100%	0	0
	lh1+so1	0	84.4%	15.6%
SQW	hh1	100%	0	0
	hh2	100%	0	0
	lh1+so1	0	64.5%	35.5%

Table 4.1 Electron and hole components in different energy states

The hh does not couple with lh and so at $k=0$ edge, since the percentage of hh is 100%. The lh and so are coupled even at $k=0$, with lh dominant. The energy states at $k \neq 0$ are also calculated and we find that the hh , lh and so are coupled together at these states, which is in agreement with the conclusion by Ridene *et al* [31] and explains the nonparabolic dispersion relations at higher k . Another significance of CQW is the energy state shift. As shown in Fig 4.9, in SQW the $hh1$, $lh1$, $hh2$ corresponds to the stated $n=1, 2, 3$, where n is the state number. However, in CQW, the state $n=2$ becomes $hh2$ rather than $lh1$. This is due to the coupling between the QWs, the wave function of $lh1$ is no longer confined simply in one QW (see Fig 4.10). Both of CQW and SQW energy levels hh , lh and so were calculated with the mentioned 8-band $k \cdot p$ model.

Figure 4.10 Comparison of wave functions between $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ CQW and SQW. The solid lines and dash lines are wave functions of CQW with different $L_b=20/60\text{\AA}$. The dot lines are wave functions of SQW.

Fig 4.11 shows the dependence of energy levels in valence band in the QW L_{z1} as a function of barrier width L_b at $k = 0$ edge. The energy levels of $hh1$ and $hh2$ change -0.1 and -1.3 meV, respectively, when L_b is increased from 20Å to 60Å. On the other hand, the $lh1$ state has an energy change of 13.3 meV. From table II and Fig 4.10 we see that the hh state does not couple with lh and so , and the wave functions are well confined in the studied QW, which means the barrier width has little effect on the hh states at $k=0$. In contrast to hh , lh has a significant energy change with increasing L_b . As L_b is increased, the interwell coupling effect is reduced and the wave function becomes more confined. What's more, when the barrier width is large enough, interwell coupling can be neglected and $lh1$ finally exceeds $hh2$ state, results in a similar case as in SQW (see Fig 4.9).

Figure 4.11 Energy dependence as a function of barrier width in $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ CQW.

The two well widths are 50 and 100Å.

Fig 4.12 shows the energy dependence as a function of well width L_{z1} . The barrier

width L_b is fixed at 30 Å and $L_{z2} = 100$ Å. As L_{z1} is increased from 30 to 110 Å, all the three energy levels increase, but an intersection happens at $L_{z1} = 46$ Å between $hh2$ and $lh1$. From Fig 4.12 we also find hh states increase faster than lh state at $L_{z1} < 110$ Å. Since the barrier width is 30 Å, interwell coupling is to be taken into account. Whereas, as shown in Fig 4.9, interwell coupling has less influence on $hh1$ and $hh2$ state than on $lh1$ state, therefore the energy levels $hh1$ and $hh2$ depends more on well width L_{z1} but not coupling effect.

Figure 4.12 Energy dependence as a function of well width L_{z1} .

Fig 4.13 shows the CQW energy diagram as function of Ge composition. In previous diagrams, the zero energy is taken as the average of bottom hh and lh bands in the strained QW. However, since the valence band offset is $\Delta E_v = 0.84x$ [42], the zero energy reference changes with changing x , therefore we use the top valence band edge of barrier (Si) as new zero reference to normalize the energy values. The x value is

increased from 0.1 to 0.6, and we find that the energy increase approximate linearly with increasing x , which indicates that the band offset has the most significant influence on the subband energy levels within different combinations of well material $\text{Si}_{1-x}\text{Ge}_x$.

Figure 4.13 Energy dependence as a function of Ge composition in well material.

The coupling effect is to be verified by experimental measurements. Although our design was based on direct intersubband transition, it was examined by interband indirect transition due to equipment limitations. But we believe that the principles are the same. Firstly, the coupling effect was verified by symmetric coupled quantum wells. Two $\text{Si}_{0.65}\text{Ge}_{0.35}$ quantum wells of the same width length 6nm was separated by 2nm Si barrier, the measured PL spectra was compared with single 6nm $\text{Si}_{0.65}\text{Ge}_{0.35}$ quantum well PL, as shown in Fig 4.14.

Figure 4.14 PL spectra of samples D6 and M3. The inset is the band structure of sample D6.

The difference between samples D6 and M3 is their barrier thickness, which is that D6 has a barrier of 2nm while M3 has a barrier of 40nm, so that M3 can be treated as single well structure. The coupling effect is supposed to be observed in D6 [43, 44]. This is because when two QWs are brought closely, such as the case of sample D6, both the conduction and valence band will split into symmetric (S) and anti-symmetric (A) states due to the interwell coupling (the inset of Fig 4.14). Hence, the band edge transition energy of sample D6 is smaller than that of sample M3. About 20meV red shift is observed in the PL spectra of samples D6 and M3.

We also tried to use asymmetric structure, in which adjacent quantum wells have

different well widths, to examine the coupling effect. Fig 4.15 shows the measure PL spectra.

Figure 4.15 PL spectra of samples D1, D2, D3, D4, D5 and M2. The inset is the band structure of the DQWs samples. Thicknesses of QW1 and QW2 are 5nm and 10nm respectively.

Samples D1-D5 are of different barrier width 3, 6, 9, 12 and 20nm, the adjacent wells QW1 and QW2 width are 5nm and 10nm, while sample M2 is a 5nm $\text{Si}_{0.65}\text{Ge}_{0.35}$ single well structure. Note that the PL spectra profiles of the DQWs samples are the same as that of sample M2. In other words, the PL signals of samples D1, D2, D3, D4 and D5 actually came from QW1 (5nm thick QW) in the DQWs. The intensity of the NP peak of QW1 in the DQWs decreases as the barrier thickness decreases. The reason is that the tunneling time depends on the thickness of the barrier. Hence, when the barrier thickness decreases, more electrons and holes will tunnel from QW1 to the

thicker well, and the luminescence from QW1 will be reduced. As described in references, there should be two NP and TO peaks that come from QW1 and QW2 respectively in the PL spectra of the DQWs. However, no QW2 related PL signal was observed in our experiment.

4.3 Triple Quantum Well Structure with Electric Field

As said in previous chapters, the investigation of optoelectronics has fallen into the terahertz (THz) part of electromagnetic spectrum. Typical quantum cascade laser emission is in the mid- to far-infrared region, which has potential applications in chemical spectroscopy, medical imaging and so on. THz QCLs based on group III-V compounds have been demonstrated by many research groups. Compared with III-V compounds, Silicon based laser has potential advantages because of its mature technology in present microelectronic industry and lower cost. However, as known, *interband* radiative photon emission is constrained by the indirect band gap of Si. The milestone of Si laser research is the demonstration of successful growth of Si/SiGe cascade and observation of electroluminescence [28], though full operation of Si laser has not been realized. In this part we show the possible QCL transition mechanism in Si/SiGe active region formed by quantum wells. The band structure of SiGe quantum wells were calculated with 8-band $k \cdot p$ method. The influence of well width and Ge composition were taken into consideration.

Triple quantum wells (TQW) structure was used widely in quantum cascade emitter

design for its high efficiency of emission compared with other designs. In the original proposal by Dehlinger et al [28], the excited heavy hole *vertical* transition states HH1-HH2 were confined in a thin $\text{Si}_{0.68}\text{Ge}_{0.32}/\text{Si}$ quantum well, with well width 4 nm. However, because of the existence of light hole state LH1 between HH1 and HH2, holes from HH2 decayed to LH1 faster thus the lifetime of HH2 state was short, compared with the requirement of population inversion. Other researchers proposed *diagonal* transition to increase the lifetime of HH2 by increasing the Si barrier width, but the optical transition matrix element was also reduced. With calculation, we found that the HH2 state can be pushed up in thicker quantum well, while LH1 state was pulled down correspondingly. In our design, the active region contains three quantum wells with different widths. If no external electric field was applied, the HH1 state of each well occupied the first three states in active region. When electric field was applied, the HH2 state of the thicker well was pushed up and the first three state becomes HH1 and HH2 from the thicker well and HH1(indicated as HH1') state of the adjacent well. *Diagonal* transition will occur between HH2-HH1', while the difference between HH1-HH2 was set to the optical phonon energy and therefore enhance the population inversion.

The 8-band $k \cdot p$ method Hamiltonian including conduction band, heavy hole, light hole and spin-orbit split-off band consists of three parts:

$$H = H_k + H_s + V_{(z)} \quad (4.5)$$

where H_k and H_s are the non-strain and strain matrix, while $V_{(z)}$ is the scalar

potential, which is the band offset in conduction or valence band. Considering the effect of external electric field, a new term was added to Hamiltonian. The modified total Hamiltonian was given by:

$$H' = H + V_{F(z)} \quad (4.6)$$

where $V_{F(z)} = -eFz$ stands for the field distribution along the growth direction. To verify our calculation, we compared our result with Dehlinger's work. We obtained the transition energy HH1-HH2 = 133meV and HH1-LH1 = 66meV, which agreed with their HH1-HH2 = 130meV and HH1-LH1 = 60meV.

Our design was shown in Fig. 4.16. The widths of the three wells in active region are 80, 45 and 60 Å, and the Si barrier between each is 20 Å. The moduli square of relevant wave functions are also shown. In Fig 4.16(a), when no external electric field is applied, there are another two hole states between HH1 and HH2 of the thicker well w_1 , which will reduce the emission efficiency. When an electric field of 50 kV/cm is applied in Fig 4.16(b), the HH2 state of w_1 is pushed up above the other two states. The energy difference between HH1 and HH2 is 53 meV, which is close to the phonon energy in SiGe compounds. The radiative transmission occurs between HH1' and HH2, with energy $\Delta E = 16$ meV, which is in far-infrared region. On the other hand, holes in HH2 states decays to HH1 state with fast speed and then tunnels into the excited state of next period, which enhance the population inversion.

Figure 4.16 Energy states in designed structure with applied electric field

Compared with Dehlinger’s design, in our design LH1 state was pulled down, therefore it will give better emission efficiency. However, LH1 state and other relevant states do exist in our structure and they are not shown in Fig 4.16. Note the band offset of valence band in SiGe is about $\Delta E_v=0.84x$, where x is the percentage of Ge. Fig 4.16 shows part of valence band confinements. Due to experiment condition

limits, we can't perform the PL measurements in this far-infrared region. Further work need to be done in future.

Chapter 5 Conclusion and Recommendations

5.1 Conclusion

In conclusion, 8-band $k \cdot p$ method was applied to calculate the band structures of Si/SiGe heterostructures, so as to provide fundamentals for QCL design. Quantum wells with well width 2~11nm and Ge composition 0.2~0.8 were investigated.

Investigations follow three steps. Firstly, the Si-Ge interdiffusion at high temperature was investigated with single quantum well structure and modified 6+2 band method. The predicted blueshift agreed well with measured PL spectra and activation energy E_a of about 1.8 eV was obtained. Thereafter, the coupling effect between adjacent thin quantum wells was investigated with coupled wells structure. The coupling effect on different energy states were shown in earlier section. After that, we studied the triple quantum wells structure and designed our structure for emission in far-infrared region. The theoretical method has been verified with literatures and gets good agreements while the experimental result is to be verified.

5.2 Recommendations for Future Work

Quantum cascade structures usually comprise hundreds of layers and each layer is typically ~2nm. Therefore, the accurate thickness control is desirable. In our experiments the samples were grown with chemical vapor deposition (CVD) method,

and the equipment was constricted with limited growth rate at 12.8nm/min, which was very high for material growth. Therefore, I suggest using molecular beam epitaxy (MBE) to grow the SiGe/Si quantum cascade structures. This is because MBE could achieve relatively better interfaces between the barriers and quantum wells, with controllable lower growth rate.

Due to the growth limit, we used wide wells in our design and experiments. Specially, in our final design, because of the large well width, the transition mechanism was identified as intrawell (vertical) transition. Interwell (diagonal) transition is also a good approach for light emission. However, diagonal transition requires very thin layer growth so that the carriers are able to penetrate the Si barriers. I suggest trying the diagonal transition with MBE growth.

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