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Study of SiGe/Si Quantum Cascade Structures

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in fulfilment of the requirement for the degree of
Master of Engineering

2007

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.

23/11/07

Date

Wang Rui

Acknowledgment

"Few people are successful unless a lot of other people want them to be"

— Charles Brower

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Table of Contents

Statement of Originality.....i

Acknowledgmentii

Table of Contentsiii

Summary v

List of Figuresvi

List of Tablesix

Chapter 1 Introduction and Motivation 1

1.1 Background..... 1

1.2 Potential Applications2

1.3 Motivation4

1.4 Challenges and Objectives5

1.5 Thesis Overview.....6

Chapter 2 Theoretical Review 7

2.1 Strain Effect on SiGe/Si Heterostructure7

2.2 Critical Thickness of SiGe/Si Heterostructure10

2.3 Strain Effect on Band Structure.....13

2.4 Quantum Cascade Structure16

Chapter 3 Fabrication and Characterization 25

3.1 Fabrication25

3.1.1 System Description26

3.1.2 Source Gases for UHV-CVD28

3.1.3 Control of Composition and Deposition Rate.....28

3.2 Characterization Tools30

Chapter 4 Results and Discussion 32

4.1 Sample of SiGe/Si Quantum Staircase Emitter33

4.2 Samples M1, M2 and M338

4.2.1 Experiments38

- 4.2.2 Results and Discussion 39
- 4.3 Samples D1, D2, D3, D4 and D5 48**
 - 4.3.1 Experiments 48
 - 4.3.2 Results and Discussion 49
- 4.4 Samples D6 and D7..... 50**
 - 4.4.1 Experiments 50
 - 4.4.2 Results and Discussion 51
- 4.5 Samples SL1 and SL2..... 59**
 - 4.5.1 Experiments 59
 - 4.5.2 Results and Discussion 60
- 4.6 Samples SLD1, SLD2, SLD3 and TQWs..... 65**
 - 4.6.1 Experiments 65
 - 4.6.2 Results and Discussion 66
- Chapter 5 Conclusion and Recommendations..... 71**
 - 5.1 Conclusion 71
 - 5.2 Recommendations for Future Work 73
- Bibliography..... 75**
- Author’s Publication 81**
- Appendix..... 82**

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. However, the indirect bandgap characteristic of silicon prohibits efficient radiative recombination of electrons and holes to result in coherent optical emission. Hence, various solutions have been tried to overcome this physical challenge. In 1994, the first quantum cascade laser (QCL), which is based on intersubband transition, was successfully demonstrated by scientists in Bell Labs. The realization of the QCL provides a promising technique to produce Si-based laser, because the transition mechanism for the QCL can avoid the indirect band property of Si and SiGe.

In this thesis, the theory and various designs of the quantum cascade structures are described. The SiGe/Si heterostructure was investigated to design a SiGe/Si quantum cascade emitter (QCE). Multiple quantum wells (MQWs), double quantum wells (DQWs) and SiGe/Si superlattice structures were grown by the ultra high vacuum chemical vapor deposition (UHV-CVD) epitaxial system at IME. Interband photoluminescence (PL) measurements were conducted on the as-grown and rapid thermal annealed samples, in which the quantum confinement effect, Ge-atom interdiffusion effect and interwell coupling effect were observed. Finally, room temperature Fourier transform infrared (FTIR) spectroscopy and low temperature (14K) optical transmission measurements were performed on the SiGe/Si superlattice structures. The current-voltage (I-V) characteristics of SiGe/Si quantum cascade structures with p-type contacts were also studied.

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. [19].	8
Figure 2.2	Plot of critical thickness vs. germanium fraction of pseudomorphic $\text{Si}_{1-x}\text{Ge}_x$ layers grown on bulk (100) silicon. The data is calculated by using the Matthews and Blakeslee's model, and it also includes a metastable curve for MBE growth at 550°C [19].	12
Figure 2.3	Degenerate band due to hydrostatic and uniaxial strain	14
Figure 2.4	Band structure of Si affected by the hydrostatic and uniaxial strain [34]	15
Figure 2.5	Schematic diagram of the conduction band of a quantum cascade laser [35]	16
Figure 2.6	Schematic diagram of the band structure and intersubband transitions in the active region of the quantum cascade structure in Figure 2.5 [35].	17
Figure 2.7	Schematic diagram of the quantum staircase structure [37]	18
Figure 2.8	E-k diagram of an inverted or negative effective mass structure [18]	21
Figure 2.9	Schematic diagram of the quantum staircase structure based on HH2 to LH1 optical transitions [18].	22
Figure 2.10	Schematic diagram of the quantum staircase structure based on interwell or diagonal transitions [18]	23
Figure 2.11	Schematic diagram of mini-band cascade structure [19]	23
Figure 3.1	Schematic diagram of the Canon Anelva I-2100SRE UHV-CVD system	27
Figure 4.1	Schematic diagram and TEM scans of the sample	34
Figure 4.2	E-k and valence band diagrams of the quantum staircase emitter [43]	35
Figure 4.3	I-V characteristics of the quantum staircase emitter at various temperatures (21, 40, 60, 80 and 100°C)	35
Figure 4.4	Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for the quantum staircase sample	37
Figure 4.5	SEM scan of the quantum staircase emitter sample	37
Figure 4.6	Schematic diagram and TEM scan of 10-period MQWs (M1)	39

Figure 4.7	Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples M1, M2 and M3 (from top to bottom)	41
Figure 4.8	Cross sectional TEM micrographs of samples (a) M1, (b) M2 and (c) M3	42
Figure 4.9	PL spectra of the as-grown samples taken at 4.2K	43
Figure 4.10	PL spectra of samples M2 and M3 measured at 5, 40 and 70K	44
Figure 4.11	PL spectra of the as-grown and annealed samples measured at 5K. (L_z is the width of the QW).....	45
Figure 4.12	TEM scans of the as-grown (left side) and annealed (right side) sample (M1)	46
Figure 4.13	PL spectra of the annealed samples (900°C) taken at 5K	47
Figure 4.14	Schematic diagram and TEM scan of five-period DQWs sample (D1)	48
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.....	49
Figure 4.16	Schematic diagrams and TEM scans of samples D6 and D7.....	51
Figure 4.17	Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples D6, D7 and M3 (from top to bottom)	52
Figure 4.18	PL spectra of samples D6, D7 and M3. The inset is the band structure of the DQWs samples. TO, TA and NP represent the transverse optical, transverse acoustic phonon-assisted and no-phonon transition, respectively.	55
Figure 4.19	Schematic diagram of the band structure of a strained $\text{Si}_{0.66}\text{Ge}_{0.34}$ layer grown on Si substrate. The values of the energies shown in the figure are calculated at 4.2K.....	56
Figure 4.20	Schematic diagrams and TEM scans of samples SL1 and SL2	60
Figure 4.21	Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples SL1 and SL2 (from top to bottom)	61
Figure 4.22	FTIR spectra of samples SL1, SL2 and a Si substrate (top). Intensity ratio of the Si substrate to the samples (bottom).....	63
Figure 4.23	Optical transmission spectra of samples SL1, SL2 and a Si substrate (top). Intensity ratio of the Si substrate to the samples (bottom).....	63
Figure 4.24	PL spectra of samples SL1 and SL2	64
Figure 4.25	Schematic diagram and TEM scan of samples SLD2.....	66
Figure 4.26	Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples SLD1, SLD2 and SLD3 (from top to bottom)	

.....67

Figure 4.27 I-V characteristics of samples SLD1, SLD2, SLD3 and TQWs68

Figure 4.28 Optical transmission spectra of samples SLD1, SLD2, SLD3, TQWs and a Si substrate (top). Intensity ratio of the Si substrate to the samples (bottom).....69

Figure 4.29 PL spectra of samples SLD1, SLD2, SLD3 and TQWs70

List of Tables

Table 1 Design of experiments and growth conditions.....32

Table 2 Parameters used in the calculations. Note: a_c , a_v and b are obtained
from Ref. 19 and other parameters are obtained from Ref. 75.58

Chapter 1 Introduction and Motivation

1.1 Background

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.

1.2 Potential Applications

Quantum cascade laser has attracted a great amount of attention since it was invented. The reason that the QCL becomes such an attractive 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 clarifying 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 laser is a very good and 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 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].

1.4 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.

1.5 Thesis Overview

In this thesis, chapter 1 describes the potential applications of the QCLs, motivation for conducting this project and the challenges faced during the experiments. The main objectives are also stated in chapter 1. In chapter 2, theoretical review on strain and its effect on the band structure of the SiGe/Si heterostructures are stated. The various designs of quantum cascade structures are also introduced in this chapter. Experiment setups and results analysis are presented in chapter 3 and chapter 4, respectively. The last chapter summarizes the thesis and gives recommendations for the future work.

Chapter 2 Theoretical Review

2.1 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 $5.43\text{\AA}$ and $5.65\text{\AA}$, 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 the materials system, $a_{||}$, $a_{A\perp}$ and $a_{B\perp}$ can be expressed by the following equations [20]:

$$a_{//} = (a_A G_A h_A + a_B G_B h_B) / (G_A h_A + G_B h_B) \quad (1)$$

$$a_{A\perp} = a_A [1 - D_A (a_{//} / a_A - 1)] \quad (2a)$$

$$a_{B\perp} = a_B [1 - D_B (a_{//} / a_B - 1)] \quad (2b)$$

In equation (1), $G_{A,B}$ 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 (1) can be reduced to $a_{//} \cong a_A$. In equation (2), $D_{A,B}$ 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]:

$$G_{A,B} = 2(c_{11}^{A,B} + 2c_{12}^{A,B}) (1 - D_{A,B} / 2) \quad (3)$$

$$D_{001} = 2(c_{12} / c_{11}) \quad (4a)$$

$$D_{110} = (c_{11} + 3c_{12} - 2c_{44}) / (c_{11} + c_{12} + 2c_{44}) \quad (4b)$$

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

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]:

$$a_{\text{Si}_{1-x}\text{Ge}_x} = 0.5431 + 0.01992x + 0.0002733x^2 \text{ (nm)} \quad (5)$$

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]:

$$\epsilon_{A,B//} = (a_{//}/a_{A,B} - 1) \quad (6)$$

$$\epsilon_{A,B\perp} = (a_{A,B\perp}/a_{A,B} - 1) \quad (7)$$

By combining equations (1) and (6) and assuming equilibrium condition, the relation between $\epsilon_{A//}$ and $\epsilon_{B//}$ (the parallel strain of layers A and B) can be expressed by the following equation:

$$\epsilon_{A//} = -\left(\frac{G_B h_B}{G_A h_A}\right) \epsilon_{B//} \quad (8)$$

This equation implies that the average strain at the parallel direction of the two layers could be zero by adjusting the layer thickness ($h_{A,B}$) and the shear moduli ($G_{A,B}$), which depend on the Ge fraction in SiGe alloy. Therefore, theoretically speaking, a superlattice structure consisting of infinite layers of strain balanced $\text{Si}_{1-x}\text{Ge}_x$ and $\text{Si}_{1-y}\text{Ge}_y$ films can be grown.

2.2 Critical Thickness of SiGe/Si Heterostructure

The critical thickness is defined as the maximum thickness of an epilayer grown on the substrate. When the critical thickness is exceeded, the accumulated strain energy due to the lattice mismatch between the Si and $\text{Si}_{1-x}\text{Ge}_x$ layers will increase significantly. Thereafter, the $\text{Si}_{1-x}\text{Ge}_x$ epilayer will be relaxed by creating defects and

forming misfit dislocations. Once the SiGe epilayer becomes strain-relaxed, its electrical, optical, and thermal properties will be significantly degraded. This is due to the defects created during relaxation.

To avoid exceeding the critical thickness, a number of models have been developed to calculate its value. A thermodynamic equilibrium model suggested by Van der Merwe [22] describes the critical thickness by analyzing the total system energy. It is expressed as follows,

$$h_c \cong \frac{19}{16\pi^2} \left(\frac{1+\nu}{1-\nu} \right) \left(\frac{b}{f} \right) \quad (9)$$

where ν represents the Poisson's ratio, b is absolute value of the Burger's vector which represents the magnitude and direction of the lattice distortion of dislocation in a crystal lattice, and f represents the misfit strain between the substrate and the epilayer.

b and f are expressed as follows:

$$b = a_s / \sqrt{2} \quad (10a)$$

$$f = \frac{a_{\text{epi}} - a_s}{a_s} \quad (10b)$$

where a_s and a_{epi} are the lattice constants of the substrate and the epilayer, respectively.

Figure 2.2 Plot of critical thickness vs. germanium fraction of pseudomorphic $\text{Si}_{1-x}\text{Ge}_x$ layers grown on bulk (100) silicon. The data is calculated by using the Matthews and Blakeslee's model, and it also includes a metastable curve for MBE growth at 550°C [19].

Another model for the critical thickness was developed by Matthews and Blakeslee [23]. The model uses an equivalent approach of balancing the forces for a propagating and threading dislocation. By balancing the force of the threading dislocation in an uncapped epilayer with the restoring tension force from the extra interfacial dislocation, the critical thickness could be obtained:

$$h_c \cong \frac{b}{2\pi f} \frac{1 - v \cos^2 \theta}{(1 + v) \cos \lambda} \left[\ln \left(\frac{h_c}{b} \right) + 1 \right] \quad (11)$$

where θ is the angle between the dislocation line and its Burgers vector, and λ is the angle between the Burger's vector and the direction in the interface perpendicular to the dislocation line. b , f , and v have the same meaning as they are in equation (9).

Figure 2.2 plots the critical thickness calculated by employing the Matthews and Blakeslee's theory vs. Ge fractions in $\text{Si}_{1-x}\text{Ge}_x$ pseudomorphically grown on a Si (100) substrate.

Houghton also produced a semi-empirical kinetic model in an extensive study. The model calculates the critical thickness for appropriate thermal treatments to metastable films grown at low temperatures [24]. The critical thickness of a strained $\text{Si}_{1-x}\text{Ge}_x$ layer grown pseudomorphically on a bulk Si (100) substrate is given by:

$$h_c \cong \frac{0.55}{x} \ln(10h_c) \cong 1.7793x^{-1.2371} (\text{nm}) \quad (12)$$

This equation is derived from equation (11) by taking the misfit strain between the pure Si and Ge, and the propagation of 60° -type misfit dislocations. According to equation (10b), $f = (a_{\text{Ge}} - a_{\text{Si}})/a_{\text{Si}} = 0.0418$. $\cos\lambda = \cos\theta = \cos 60^\circ = 0.5$ for 60° -type misfit dislocations [19,25].

2.3 Strain Effect on Band Structure

SiGe/Si heterostructures allow both strain and bandgap engineering using silicon technology. It is important for designers to understand how strain affects the band structure of the SiGe/Si materials system. A series of papers have been published by Van de Walle [20,26-29] and People [30-33], which calculate the band structure of the SiGe/Si hetero-system. In their work, both the self-consistent pseudopotential and k·p method were involved. However, in this section, the band structure described is

calculated by the self-consistent pseudopotential method.

The band structure of the SiGe/Si heterostructure is affected by both hydrostatic and uniaxial strain, which are expressed graphically in Figure 2.3. The hydrostatic strain is due to the change in the volume of the material. It results in energy shifts in both the conduction and valence band, which can be expressed as follows [28]:

$$\Delta E_{c,av} = a_c \frac{\Delta\Omega}{\Omega} = a_c (2\varepsilon_{//} + \varepsilon_{\perp}) \quad (13a)$$

$$\Delta E_{v,av} = a_v \frac{\Delta\Omega}{\Omega} = a_v (2\varepsilon_{//} + \varepsilon_{\perp}) \quad (13b)$$

where a_c and a_v are the hydrostatic deformation potential for the conduction and valence band, respectively. $\Delta\Omega/\Omega$ is the fractional volume change, and it is the sum of ε_{xx} , ε_{yy} and ε_{zz} . ε_{xx} and ε_{yy} are strains along x and y axis, respectively. They are equal to each other, hence they are defined as $\varepsilon_{//}$. ε_{zz} is defined as $\varepsilon_{\perp}$, which is the strain along the growth direction.

Figure 2.3 Degenerate band due to hydrostatic and uniaxial strain

The uniaxial strain splits both the degenerate conduction and valence band, as shown in Figure 2.3. In the conduction band, the uniaxial strain along the (001) direction splits the bands along the (100) and (010) directions from that along the (001) direction. The resulting energy shifts of the conduction bands are given by [20]:

$$\Delta E_c^{001} = \frac{2}{3} \Xi_u^\Delta (\epsilon_\perp - \epsilon_\parallel) \quad (14)$$

$$\Delta E_c^{100,010} = -\frac{1}{3} \Xi_u^\Delta (\epsilon_\perp - \epsilon_\parallel) \quad (15)$$

where Ξ_u is the uniaxial strain deformation potential for the conduction band. The energy splitting of the valence bands is given by [20]:

$$\Delta E_{v,1} = -\frac{1}{6} \Delta_0 + \frac{1}{4} \delta E + \frac{1}{2} \left[\Delta_0^2 + \Delta_0 \delta E + \frac{9}{4} (\delta E)^2 \right]^{1/2} \quad (16)$$

$$\Delta E_{v,2} = \frac{1}{3} \Delta_0 - \frac{1}{2} \delta E \quad (17)$$

$$\Delta E_{v,3} = -\frac{1}{6} \Delta_0 + \frac{1}{4} \delta E - \frac{1}{2} \left[\Delta_0^2 + \Delta_0 \delta E + \frac{9}{4} (\delta E)^2 \right]^{1/2} \quad (18)$$

where Δ_0 is the spin-orbit splitting. For strain along the (001) direction, δE is equal to $2b(\epsilon_\perp - \epsilon_\parallel)$, where b is the uniaxial deformation potential for tetragonal strain. $\Delta E_{v,1}$, $\Delta E_{v,2}$ and $\Delta E_{v,3}$ represent the band energy offsets of the light, heavy and split-off band at the valence band, respectively. Figure 2.4 shows the band energy shifts between unstrained and strained Si. The terms on the left-side of equations (13-18) are labeled in the figure.

Figure 2.4 Band structure of Si affected by the hydrostatic and uniaxial strain [34]

2.4 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 2.5 Schematic diagram of the conduction band of a quantum cascade laser [35]

Figure 2.6 Schematic diagram of the band structure and intersubband transitions in the active region of the quantum cascade structure in Figure 2.5 [35].

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 2.5 [35]. It is composed of two parts: the active and injector regions. The injector region is formed by a chirped superlattice structure, where the mini-band is formed. The active region can be illustrated in Figure 2.6. It is a four level system (it is also considered as a three level system in some literature, because energy level E_0 is E_0' in the adjacent downstream active region). The carriers coming from energy level E_0' tunnel across the barrier into energy level E_2 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_1 , then to energy level E_0 . In order to achieve the population inversion in the active region, the lifetime for transition from E_1 to E_0 must be significantly less than the lifetime for transition from E_2 to E_1 . This could be realized by designing the energy separation of energy level E_1 and E_0 to be resonant with the optical phonon energy in

the host material. At the same time, the transition from E_2 to E_1 must involve significant momentum transfer in terms of optical phonon emission, so that the lifetime for transition from E_2 to E_1 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_0 becomes resonant with the energy level E_2 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 2.7 Schematic diagram of the quantum staircase structure [37]

A second design (as shown in Figure 2.7) was firstly proposed by Friedman *et al.* [37,38]. It is relatively simpler than the previous one. The structure comprises injector, active region and collector. The active region has been prepared 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 HH1 to LH1 transitions. 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 [37]:

$$F = E_{\text{LH-HH}}/(w + b) \quad (19)$$

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 [37,39], as shown in Figure 2.8. 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 2.8. 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 2.8 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 2.9. 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 2.9 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 2.10. 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 2.10 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 [40]. 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 2.11 Schematic diagram of mini-band cascade structure [19]

Among the various designs of the quantum cascade structures, the design shown in Figure 2.5 has been proved feasible in the III-V materials system [41]; furthermore, the intersubband electroluminescence from the SiGe/Si materials system has been demonstrated using this design [42]. However, the growth of quantum staircase structure, which is shown in Figure 2.7, is relatively easier, and the structure with relatively low Ge fraction ($<30\%$) has been proved feasible as well [43,44]. Therefore, the quantum staircase structure was studied in our project.

Chapter 3 Fabrication and Characterization

3.1 Fabrication

The first epitaxy of $\text{Si}_{1-x}\text{Ge}_x$ layers was achieved using molecular beam epitaxy [45], and many universities still use MBE systems in research. In industry, chemical vapour deposition (CVD) systems are used for $\text{Si}_{1-x}\text{Ge}_x$ epitaxy. There are a number of main reasons for the dominance of CVD in production and industrial environments. The first is historical reason. Silicon epitaxy has employed atmospheric CVD with silane (SiH_4) or a silicon halide ($\text{SiH}_{4-z}\text{Cl}_z$ with $1 \leq z \leq 4$) at high temperatures since the 1960s [46]. The second is the control of particulate density. The drive in the semiconductor industry has resulted in readily available and high-purity gas sources for Si epitaxy. For high yield CMOS or bipolar production using lithographic techniques, the particulate density must be as close to zero as possible. Solid source MBE has the disadvantage that material is deposited on the walls of the growth chamber which over time can fall off and create particles. Therefore, there have been large investments on developing CVD reactors for production. Hence CVD has the uniformity and reproducibility required for high yield production through the larger investments in the technology.

A number of different CVD reactors have been developed for the low temperature growth of strained $\text{Si}_{1-x}\text{Ge}_x$ films. These can be conveniently divided into ultra-high

vacuum CVD (UHV-CVD) at growth pressures of less than 10 Pa [47-50] and low pressure CVD (LPCVD) with pressures ranging from 10 to 1000 Pa [51]. In this study, the Canon Anelva I-2100SRE UHV-CVD system is used.

3.1.1 System Description

Figure 3.1 shows the schematic diagram of the Canon Anelva I-2100SRE UHV-CVD system in IME. The system mainly consists of two load-locks (sample entry chamber), a transfer module and a process module (reaction chamber). The load-locks and transfer module are shown in the left portion of Figure 3.1, while the process module is shown in the right portion of the figure. The load-locks are pumped with a turbo molecular pump and a rough pump to a base pressure of 0.1 Pa. The transfer module mainly comprises a transfer chamber, an aligner and an incooler system. The transfer chamber is pumped by a molecular pump and a rough pump to a base pressure of 10^{-9} Pa. This chamber serves as a vacuum buffer between the sample entry and the reaction chamber. Magnetically coupled transfer arms are used to transfer samples between the chambers. The aligner system is used to equalize wafer alignment. It shares the same exhaust system with the transfer chamber. The incooler system is used for cooling the processed wafer. When the incooler system is operating, a poppet valve isolates the incooler system from the transfer chamber. After the cooling process is finished, the incooler system is pumped to certain vacuum before the poppet valve opens.

Figure 3.1 Schematic diagram of the Canon Anelva I-2100SRE UHV-CVD system

The process module is connected to the transfer chamber through the connecting port. Its main part is a process chamber, which is a single-wafer ultra vacuum CVD chamber. The process chamber is composed of a growth chamber where process gas is introduced into and a heater chamber equipped with substrate heating mechanism. Each chamber is pumped by a turbo molecular pump. The Si substrate is heated from the backside in the heater chamber. The wall of the growth chamber and the shroud of the heater chamber are water cooled. The purpose is to confine gas decomposition only on the surface of the substrate.

3.1.2 Source Gases for UHV-CVD

Normally, source gases of the UHV-CVD epitaxial system for growing the SiGe/Si heterostructures include SiH₄, disilane (Si₂H₆), dichlorosilane (DCS or SiH₂Cl₂) and germane (GeH₄). P-type doping is achieved by using diborane (B₂H₆), while arsine (AsH₃) or phosphine (PH₃) is used for n-type doping. SiH₂Cl₂ has also been used extensively for the selective epitaxial growth [52]. The selective growth with SiH₄ is more difficult. However, differential growth is quite common in SiH₄ chemistries. The single crystal Si material is grown in the oxide windows, while the poly- or amorphous-silicon is grown on top of any oxide. The poly- or amorphous-silicon can be easily etched away. Therefore SiH₄ chemistry can be used for the selective deposition when combined with the selective etching techniques. In this Anelva epitaxial system, gas source Si₂H₆ and GeH₄ are used to grow the SiGe/Si heterostructures, while B₂H₆ and PH₃ are used for p- and n-type doping, respectively.

3.1.3 Control of Composition and Deposition Rate

The surface reactions of Si₂H₆ and GeH₄ depend on the Si and Ge composition and also on the surface orientation. Now, assuming that Si₂H₆ and GeH₄ are adsorbed at adsorption sites, according to the Langmuir adsorption isotherm and decompose, the Si₂H₆ and GeH₄ reaction rates, R_{Si} and R_{Ge} (cm/min), are given by the following equations [53-55]:

$$R_{Si} = \frac{k_{Si}[k_1/(k_{Si} + k_{-1})]P_{Si_2H_6}n_0}{1 + [k_1/(k_{Si} + k_{-1})]P_{Si_2H_6} + [k_2/(k_{Ge} + k_{-2})]P_{GeH_4}} \quad (20)$$

$$R_{Ge} = \frac{k_{Ge}[k_2/(k_{Ge} + k_{-2})]P_{GeH_4}n_0}{1 + [k_1/(k_{Si} + k_{-1})]P_{Si_2H_6} + [k_2/(k_{Ge} + k_{-2})]P_{GeH_4}} \quad (21)$$

where k_{Si} and k_{Ge} are the Si_2H_6 and GeH_4 reaction rate constants, and k_1 and k_2 are the Si_2H_6 and GeH_4 adsorption rate constants, respectively. The expressions of $k_1/(k_{Si}+k_{-1})$ and $k_2/(k_{Ge}+k_{-2})$ denote the Si_2H_6 and GeH_4 adsorption equilibrium constants, respectively. n_0 is the total adsorption site density, and $P_{Si_2H_6}$ and P_{GeH_4} are the Si_2H_6 and GeH_4 partial pressures, respectively. The GeH_4 reaction rate in pure Ge deposition is nearly proportional to the GeH_4 partial pressure, while the Si_2H_6 reaction rate in pure Si deposition is not strongly dependent on the Si_2H_6 partial pressure under the similar deposition. Hence, it is expected that $[k_1/(k_{Si}+k_{-1})]P_{Si_2H_6} \gg [k_2/(k_{Ge}+k_{-2})]P_{GeH_4}$ in the above two equations. In other words, the density of the adsorbed Ge hydrides is negligibly small compared with the total adsorption site density, but the density of the adsorbed Si hydrides cannot be neglected under the investigated conditions. Assuming $k_{Si} \gg k_{-1}$ and $k_{Ge} \gg k_{-2}$, we can obtain:

$$R_{Si} = \frac{k_1 P_{Si_2H_6} n_0}{1 + (k_1/k_{Si}) P_{Si_2H_6}} \quad (22)$$

$$R_{Ge} = \frac{k_1 P_{GeH_4} n_0}{1 + (k_1/k_{Ge}) P_{GeH_4}} \quad (23)$$

Hence, the Ge fraction x is given by

$$x = \frac{R_{Ge}}{R_{Si} + R_{Ge}} = \frac{k_2}{k_1} \frac{P_{GeH_4}}{P_{Si_2H_6} + (k_2/k_1) P_{GeH_4}} \quad (24)$$

Following these equations, the growth rate and Ge composition could be controlled. However, the above equations are only theoretical formulae. Calibrations have to be done in a real system.

3.2 Characterization Tools

Several characterization tools were involved in this project. Photoluminescence (PL) spectroscopy is the most useful one. It is a classical optical tool for the characterization of semiconductors. It provides information both about the intrinsic optical processes in the host semiconductor and the extrinsic optical processes associated with impurities and defects which are inherent in practical semiconductor materials. The PL system used in this project mainly comprises an argon laser source, a refrigeration system cooled by compressed helium, a lock-in amplifier and a liquid nitrogen cooled Ge detector. Samples are mounted to a holder located in the refrigeration system and irradiated by the laser source through a chopper. The emission light goes through a monochromator, and then it is detected by the Ge detector.

X-ray diffraction (XRD) technique and cross sectional transmission electron microscopy (XTEM) were also used to analyze the Ge fraction and microstructure of the SiGe/Si heterostructures. XRD is a technique that has been used extensively for evaluating the composition and state of relaxation in the SiGe alloy layers. It is also used to characterize the quality of SiGe superlattice layers. The layers in the superlattice act as artificial planes for Bragg diffraction and produce a series of peaks in the low angle 2θ region. The positions of peaks can be approximated from Bragg's law [56]:

$$n\lambda = 2d \sin\theta \quad (25)$$

where λ is the x-ray wavelength, d is the layer thickness, θ is the angle between the lattice planes and the incident x-ray beam and n is an integer that indicates the order of the reflection. In our system, a simulation software was installed. By adjusting the input parameters, such as the Ge fraction and the thicknesses of epilayers, a simulated XRD spectrum that fits the scanned XRD rocking curve nicely can be obtained. Hence the Ge fractions can be determined.

Cross sectional transmission electron microscopy can image interfaces and structures at very high resolution and allow characterization of SiGe superlattice layers through the identification of defects. As such, it compliments the XRD measurement, which is sensitive to the level of defects but cannot identify their microscopic nature.

Chapter 4 Results and Discussion

The table below shows the structures and growth conditions of the samples investigated in this project. Detail analysis of these samples will be described in the following sections.

Table 1 Design of experiments and growth conditions

Sample name	Type	No. of periods	QWs (nm)	Barrier (nm)	Spacing layer (nm)	Doping conc. (cm^{-3})	Growth temp. ($^{\circ}\text{C}$)
QCE	Quantum cascade structure	20	4.9	3	—	10^{19}	530
M1	MQWs	10	4	40	—	—	530(QWs) 600(barriers)
M2	MQWs	10	5	40	—	—	
M3	MQWs	10	6	40	—	—	
D1	Asymmetric DQWs	5	5 (QW1) 10(QW2)	3	40	—	530(QWs and barriers) 600(spacing layers)
D2	Asymmetric DQWs	5	5 (QW1) 10(QW2)	6	40	—	
D3	Asymmetric DQWs	5	5 (QW1) 10(QW2)	9	40	—	530(QWs)
D4	Asymmetric DQWs	5	5 (QW1) 10(QW2)	12	40	—	600(barriers and spacing layers)
D5	Asymmetric DQWs	5	5 (QW1) 10(QW2)	20	40	—	
D6	Symmetric DQWs	5	6	2	40	—	530(QWs and barriers) 600(spacing layers)
D7	Symmetric DQWs	1	6	4	—	—	
SL1	Superlattice	5	6	2	—	—	530
SL2	Superlattice	10	6	4	—	—	
SLD1	Superlattice	5	6	2	—	10^{19}	530(QWs and barriers) 600(spacing and contact layers)
SLD2	Superlattice	15	6	2	100	10^{19}	
SLD3	Superlattice	15	5	3	100	10^{19}	
TQWs	Triple QWs	3	8 (QW1) 4.5(QW2) 6 (QW3)	2	100	10^{19}	

4.1 Sample of SiGe/Si Quantum Staircase Emitter

The structure of SiGe/Si quantum staircase emitter was designed according to reference [43]. The schematic diagram and cross sectional TEM scans of this structure are shown in Figure 4.1. The E-k and valence band diagrams are shown in Figure 4.2, the intersubband transitions are expected to occur inside quantum wells between the energy band of LH1 and HH1.

The growth was done at 530°C by employing the UHV-CVD system described in section 3.1.1. The reactant gases used for the deposition of the $\text{Si}_{1-x}\text{Ge}_x$ epilayers are Si_2H_6 and GeH_4 . The substrate is a p-type (boron doped at $2.5 \times 10^{15} \text{ cm}^{-3}$) Si (100) wafer with a $\text{Si}_{0.75}\text{Ge}_{0.25}$ strain relaxation buffer, which consisted of approximately 2 μm of graded SiGe (the Ge fraction is graded from 0% to 25%) following by 1 μm of $\text{Si}_{0.75}\text{Ge}_{0.25}$ buffer layer. The substrate was cleaned using a standard solution comprising 10DI:2H₂O₂:1NH₄OH (by volume), then dipped into dilute HF (DHF) solution comprising 200H₂O:1HF for 2 minutes before deposition. The active layers were strain balanced on top of the $\text{Si}_{0.75}\text{Ge}_{0.25}$ strain relaxation buffer. A 200nm $\text{Si}_{0.75}\text{Ge}_{0.25}$ contact layer was grown before 15nm graded SiGe injector layer. The active region comprising 20 periods of 3nm Si barriers and 4.9nm $\text{Si}_{0.6}\text{Ge}_{0.4}$ quantum wells was grown on the graded SiGe injector layer. The wafer was then capped with 3nm Si and 15nm graded SiGe collector layers. Thereafter a 40nm $\text{Si}_{0.75}\text{Ge}_{0.25}$ top

contact layer was grown. Both the bottom and top contacts are *in situ* doped by boron. The doping concentration is 10^{19}cm^{-3} .

Figure 4.1 Schematic diagram and TEM scans of the sample

Figure 4.2 E-k and valence band diagrams of the quantum staircase emitter [43]

Figure 4.3 I-V characteristics of the quantum staircase emitter at various temperatures (21, 40, 60, 80 and 100°C)

The principle of quantum cascade emitter relies heavily on the basic quantum mechanical principle of resonant tunneling, which occurs when two energy states on

both sides of a potential energy barrier have the same energy. Therefore, the tunneling effect could be obtained when the quantum staircase sample is under the influence of an electric field. The current-voltage (I-V) characteristics of the quantum staircase sample measured at various temperatures (21, 40, 60, 80 and 100°C) are shown in Figure 4.3. Aluminum ohmic contacts were made on the sample by E-beam evaporation before the I-V measurements. However, the intersubband resonant tunneling was not observed from the I-V characteristics curves. The sample has a similar characteristic as a resistor does. This is because the quantum cascade structure is a p-i-p structure, where the i-layer has a background doping concentration of 10^{16}cm^{-3} in our system. Therefore, the device with quantum cascade structure will not have an obvious junction effect [3,5]. Thereafter, intersubband EL (electroluminescence) and interband PL measurements were conducted on this sample at 14K and 5K respectively, but no SiGe related luminescence signals were detected.

The unsuccessful demonstration of intersubband transition is mainly caused by the bad crystal quality, which is proved by the XRD scan (as shown in Figure 4.4). The broad peaks in the rocking curve imply that interfaces between the quantum wells and barriers are not well formed. The cross sectional TEM micrographs in Figure 4.1 also show the unclear interfaces. In the TEM micrographs, the bright and dark regions correspond to the Si and SiGe layers respectively. The discontinuity of the Si barrier was observed in the TEM scan of the bottom 5-period SiGe/Si layers. The TEM micrographs of the top 5-period SiGe/Si layers show even unclear interfaces. The

rough interfaces in the SiGe/Si heterostructures is caused by the growth condition, which was not fully optimized at that time. There are severe dislocations of the sample, which were observed by the optical microscope and the scanning electron microscope (SEM) at the surface of the wafer (as shown in Figure 4.5). The dislocations are extended from the relaxed virtual substrate. Therefore, Si substrates were used in next experiment to avoid the uncertainty of the virtual substrates.

Figure 4.4 Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for the quantum staircase sample

Figure 4.5 SEM scan of the quantum staircase emitter sample

4.2 Samples M1, M2 and M3

4.2.1 Experiments

As described in the previous section, the experiment for creating the emission device according to reference [43] did not succeed. Therefore, the property of SiGe quantum wells, which are the essential components of the QC structure, was studied as the initial step to realize a quantum cascade emitter. In this experiment, $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ multiple quantum wells (MQWs) with different well widths were designed to study the quantum confinement effect [57]. Rapid thermal annealing (RTA) was also conducted on these samples to investigate the interdiffusion effect and the enhancement of the PL spectra [58,59]. These 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 Si_2H_6 and GeH_4 were used as source gases to grow the SiGe epilayers on the (100) p-type Si substrates. In total, three samples (M1, M2 and M3) were grown. Each sample comprises 10 periods of $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_z = 4, 5, 6\text{nm}$)/Si ($L_b = 40\text{nm}$) layers and 10nm Si capping layers (as shown in Figure 4.6). These samples were characterized by the cross sectional TEM and high resolution XRD (HR-XRD).

Figure 4.6 Schematic diagram and TEM scan of 10-period MQWs (M1)

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 were 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.

4.2.2 Results and Discussion

High resolution XRD measurements were conducted to analyze the material quality and the compositions of samples M1, M2 and M3. The experimental and simulated XRD rocking curves are show in Figure 4.7. 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. For sample M1, the simulation was performed based on a 10-period 4nm-thick Si_{0.65}Ge_{0.35} QW and 40nm-thick Si barrier stack. For sample M2,

the simulation was performed based on a 10-period 4.8nm-thick $\text{Si}_{0.63}\text{Ge}_{0.37}$ QW and 40nm-thick Si barrier stack, while the simulation of sample M3 was performed based on a 10-period 5.7nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW and 40nm-thick Si barrier stack. As shown in Figure 4.7, 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 Figure 4.8). For sample M1, the diffusion of Si into the SiGe QWs is quite obvious. Samples M2 and M3 also have the similar features, which cause the rough interfaces between the QWs and barriers and create the interfacial defects. Sample M1 has the thinnest QWs among the three samples, thus the influence of the rough interfaces and the defects will gravely affect the material quality of sample M1. Therefore, in the PL spectroscopy measurements, sample M1 has a very weak signal.

Figure 4.7 Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples M1, M2 and M3 (from top to bottom)

Figure 4.8 Cross sectional TEM micrographs of samples (a) M1, (b) M2 and (c) M3

The PL spectra of the three as-grown samples measured at 5K are shown in Figure 4.9. The peaks that correspond to energies higher than 1eV are silicon related [60]. There is an obvious peak and a wide shoulder at the extreme left in the PL spectra of samples M2 and M3. The peak is due to the no-phonon (NP) transition in alloy disorder scattering, and the shoulder is due to the transverse-optic (TO) phonon-assisted transition [61,62]. There is a certain energy shift between the NP signals of samples M2 and M3, which indicates the quantum confinement effect. The

signals of sample M1 are too weak to be distinguished. This is due to the rough interfaces and high density of defects in the fully strained QWs, as discussed in last section. For samples M2 and M3, the temperature dependency of PL spectroscopy was also studied. The PL spectra of samples M2 and M3 measured at 5K, 40K and 70K are shown in Figure 4.10. According to Vashini formula, redshift of 4meV is supposed to be observed as the temperature of the measurement environment increases from 5K to 70K. However, comparing with the FWHM of the PL spectra, the energy shift of 4meV is quite small. Therefore, we could not clearly observe the redshifts of the PL spectra in Figure 4.10. The intensities of PL signals, especially the silicon related PL signals decrease dramatically when the measurement temperature reaches 70K. The reduction of the PL intensity is due to the lattice vibration.

Figure 4.9 PL spectra of the as-grown samples taken at 4.2K

Figure 4.10 PL spectra of samples M2 and M3 measured at 5, 40 and 70K

Figure 4.11 shows the PL signals of samples M1, M2 and M3 (from top to bottom) before and after annealing (750, 800, 850 and 900°C for 100s). The blueshifts of the NP and TO peaks are caused by the Si-Ge atomic interdiffusion across the interfaces of the QWs [63]. Referring to Figure 4.12, the TEM scans of the annealed sample show that the widths of the QWs were broadened. The enhancement of the PL

intensity is due to the reduction of the density of the defects [64].

Figure 4.11 PL spectra of the as-grown and annealed samples measured at 5K. (L_z is the width of the QW)

Figure 4.12 TEM scans of the as-grown (left side) and annealed (right side) sample (M1)

Following reference [64], after annealing, the composition of the Ge atom (x') can be determined by the equation as follows:

$$x'(z, t) = \frac{x}{2} \left[\operatorname{erf} \left(\frac{L_z + 2z}{4\sqrt{Dt}} \right) + \frac{L_z - 2z}{4\sqrt{Dt}} \right] \quad (26)$$

where z is the length along the growth direction ($z=0$ at the centre of the QWs), t is the diffusion time, x is the Ge fraction in the QWs before annealing, L_z is the width of the QW, and D is the diffusion coefficient, which depends on the annealing temperature. After determining x' , the NP line energy of the $\text{Si}_{1-x'}\text{Ge}_{x'}$ at 4.2K can be expressed as follows [65]:

$$E_{\text{NP}}(x') = 1.155 - 0.874x' + 0.376x'^2 \text{ (eV)} \quad (27)$$

Figure 4.13 shows the PL spectra of the three samples annealed at 900°C for 100s. The located energies of the NP and TO peaks increase as the width of the QW decreases. The obvious energy shifts show the quantum confinement effect of the samples annealed at 900°C for 100s.

Figure 4.13 PL spectra of the annealed samples (900°C) taken at 5K

In summary, the quantum confinement effect among these MQWs samples is resolved. The interdiffusion effect of these samples is observed clearly for various annealing temperature, and the quantum confinement effect in the three samples become more obvious after 900°C annealing. Among the as-grown samples, sample M1 has poor crystal quality and optical performance due to the constraints of the growth system. Samples M2 and M3 give relatively strong PL signals, thus the QWs with widths larger than 4nm will be investigated in the future experiments.

4.3 Samples D1, D2, D3, D4 and D5

4.3.1 Experiments

Figure 4.14 Schematic diagram and TEM scan of five-period DQWs sample (D1)

In section 4.2, we confirm that the QWs grown by our UHV-CVD system are well formed when the widths of the QWs are larger than 4nm. Therefore, double quantum wells (DQWs) structures were designed to investigate the interwell coupling effect [66,67], which plays an essential role to determine the energy transitions and resultant optical and electronic properties of the SiGe/Si QC structure. In other words, the intersubband transitions in the QC structures rely on the interwell coupling in the QWs. This is because the wave functions in the QC structures are no longer confined to a single well, but penetrate into barriers and extend over the entire region. Therefore, the study of interwell coupling effect in the QWs remains a critical issue for realizing the QCE.

The $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ DQWs were grown by the UHV-CVD system under the same condition described in section 4.2.1. In total, seven samples (D1, D2, D3, D4, D5, D6 and D7) were grown. Samples D1 to D5 comprise five periods of DQWs. Each period comprises two $\text{Si}_{0.6}\text{Ge}_{0.4}$ QWs, the widths of which are 5 and 10nm, respectively. Between the two QWs is a Si barrier, the thickness of which is 3, 6, 9, 12 and 20nm for samples D1, D2, D3, D4 and D5, respectively. There is a 40nm Si spacing layer between each period of the DQWs. A 10nm Si capping layer was grown after growing the last period of DQWs (as shown in Figure 4.14). Samples D6 and D7 will be analyzed in detail in the next section.

4.3.2 Results and Discussion

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.

The PL spectra of samples D1, D2, D3, D4, D5 and M2 are shown in Figure 4.15. 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 come 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 QW (QW2), and the luminescence from QW1 will be reduced [66]. As described in references [68-70], 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. The reason for this is still unclear.

4.4 Samples D6 and D7

4.4.1 Experiments

Samples D6 and D7 were grown with the five DQWs samples described in the previous section. Sample D6 comprises 5 periods of $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_{z1} = 6\text{nm}$)/Si ($L_b = 2\text{nm}$) / $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_{z2} = 6\text{nm}$) layers. The Si spacing and capping layers are the same as other DQWs samples. Sample D7 comprises a single period of $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_{z1} = 6\text{nm}$)/Si ($L_b = 2\text{nm}$) / $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_{z2} = 6\text{nm}$) layers and 10nm Si capping layer. The schematic diagrams and TEM scans of samples D6 and D7 are given in Figure 4.16.

Figure 4.16 Schematic diagrams and TEM scans of samples D6 and D7

4.4.2 Results and Discussion

To study the interwell coupling effect of Samples D6 and D7, we compare their characteristic results with that of sample M3. The main difference of these samples is their barrier thickness. Samples D6 and D7 have 2nm and 4nm barriers respectively, while sample M3 has 40nm barriers. The thick barriers in sample M3 will effectively isolate the QWs in the sample, thus the QW in sample M3 could be considered as single QW (SQW).

Figure 4.17 Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples D6, D7 and M3 (from top to bottom)

Figure 4.17 shows the x-ray rocking curves of samples D6, D7 and M3. The sharp peaks 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. For sample D6, the simulation was performed based on a 5-period 5.6nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW, 2nm-thick Si barrier, and 5.6nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW and 40nm-thick Si barrier stack. For sample D7, the simulation was performed based on a 5.7nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW, 4nm-thick Si barrier and 5.7nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW. Finally for sample M3, the simulation was performed based on a 10-period 5.7nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW and 40nm-thick Si barrier stack. As shown in the figure, 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 are shown in Figure 4.16.

The high degree of strain (up to 1.5%) between the QWs and barriers gave rise to substantial thickness variations (the roughness is about $7\text{\AA}$) in the QWs and barriers. The thickness variations in the QWs and barriers result in the relatively weak and broad PL spectra of the SiGe QWs observed in samples D6, D7, and M3, as shown in Figure 4.18. In the figure, NP, TA and TO refers to no-phonon, transverse-acoustic phonon-assisted and transverse-optical phonon-assisted transitions, respectively [62]. The full-width at half maximum (FWHM) of the PL signal of sample M3 is about 40meV (as marked in Figure 4.18). The contribution to the FWHM of this signal by

interface roughness (ΔL) could be estimated by the following equations [71,72]:

$$\Delta E = \left[\frac{dE_{le}}{dL} + \frac{dE_{lhh}}{dL} \right] \Delta L \quad (28)$$

$$\frac{dE_{le}}{dL} = \frac{E_{le}}{\frac{L}{2} + \frac{\hbar}{\sqrt{2m_e^B(\Delta E_c - E_{le})}} \cos^2 \left(\frac{L}{2} \sqrt{\frac{2m_e^W E_{le}}{\hbar^2}} \right) + \frac{\hbar}{\sqrt{8m_e^W E_{le}}} \sin \left(L \sqrt{\frac{2m_e^W E_{le}}{\hbar^2}} \right)} \quad (29)$$

$$\frac{dE_{lhh}}{dL} = \frac{E_{lhh}}{\frac{L}{2} + \frac{\hbar}{\sqrt{2m_{hh}^B(\Delta E_v - E_{lhh})}} \cos^2 \left(\frac{L}{2} \sqrt{\frac{2m_{hh}^W E_{lhh}}{\hbar^2}} \right) + \frac{\hbar}{\sqrt{8m_{hh}^W E_{lhh}}} \sin \left(L \sqrt{\frac{2m_{hh}^W E_{lhh}}{\hbar^2}} \right)} \quad (30)$$

where L is the QW width and E_{le} and E_{lhh} are the energy values of the first energy state in the conduction and valence bands. m_e^B , m_e^W , m_{hh}^B and m_{hh}^W are the effective mass of the electron and heavy hole in the QW (W) and barrier (B), and ΔE_c and ΔE_v are the band offsets of the conduction and valence bands, respectively. Equations (29) and (30) are derived from the finite barrier model, which is accurate enough for sample M3 whose barriers are as thick as 40nm. Hence, by applying the above equations, out of the total FWHM of 40meV, 13.1meV is contributed by the interface roughness between the QW and barrier layers. The large difference of ~27meV between the estimated and measured FWHM values could be due to the presence of interface defects, which are caused by the partial strain relaxation due to lattice mismatch at the interface.

Figure 4.18 PL spectra of samples D6, D7 and M3. The inset is the band structure of the DQWs samples. TO, TA and NP represent the transverse optical, transverse acoustic phonon-assisted and no-phonon transition, respectively.

In Figure 4.18, the PL peaks shift to lower energy following decrease in the barrier thickness. This is due to the effect of interwell coupling between the two symmetrically-aligned wells caused by the wavefunction penetration across the Si barrier. When two quantum wells are brought close enough, such as the case of samples D6 and D7, the energy states in both the conduction and valence bands are split into symmetric (S) and anti-symmetric (A) states due to the coupling effect (as shown in the inset of Figure 4.18) [66]. In the valence band, both the heavy hole (HH) and light hole (LH) states are split. However, the energy of the HH S-state is higher than that of the LH S-state. Hence, the observed luminescence should be attributed to the optical transition between the S-states of electrons and the HH states in the

valence band.

Figure 4.19 Schematic diagram of the band structure of a strained Si_{0.66}Ge_{0.34} layer grown on Si substrate. The values of the energies shown in the figure are calculated at 4.2K.

In sample M3, since the thickness of the Si barrier is 40nm, the QWs in this sample should be effectively isolated from each other. This being the case, it should have similar characteristic as a single QW with the same QW width and Ge composition. The band structure of a strained Si_{0.66}Ge_{0.34} SQW grown on Si substrate is shown in Figure 4.19. For a strained Si_{1-x}Ge_x layer ($x < 0.4$) grown on Si substrate, the indirect bandgap E_g at 4.2K can be expressed as [65]:

$$E_{g, \text{SiGe}}(x) = 1.17 - 0.896x + 0.396x^2 \text{ (eV)} \quad (31)$$

The valence band discontinuity is given by the following equation [19]:

$$\Delta E_v = 0.74x \text{ (eV)} \quad (32)$$

Hence the conduction band offset could be obtained by:

$$\Delta E_c = -0.156x + 0.396x^2 \quad (33)$$

If the value of ΔE_c is positive, the band alignment is type-II, otherwise the band alignment is type-I. According to the work of Van de Walle and Martin [20,28], the energy splitting of the valence and conduction bands are given by the following equations:

$$\Delta E_c^{001} = \frac{2}{3} \Xi_u^A (\epsilon_{\perp} - \epsilon_{\parallel}) \quad (14)$$

$$\Delta E_c^{100,010} = -\frac{1}{3} \Xi_u^A (\epsilon_{\perp} - \epsilon_{\parallel}) \quad (15)$$

$$\Delta E_{v,1} = -\frac{1}{6} \Delta_0 + \frac{1}{4} \delta E + \frac{1}{2} \left[\Delta_0^2 + \Delta_0 \delta E + \frac{9}{4} (\delta E)^2 \right]^{1/2} \quad (16)$$

$$\Delta E_{v,2} = \frac{1}{3} \Delta_0 - \frac{1}{2} \delta E \quad (17)$$

$$\Delta E_{v,3} = -\frac{1}{6} \Delta_0 + \frac{1}{4} \delta E - \frac{1}{2} \left[\Delta_0^2 + \Delta_0 \delta E + \frac{9}{4} (\delta E)^2 \right]^{1/2} \quad (18)$$

The detail explanations of these equations are present in section 2.3. A finite barrier model was established based on the above equations and Schrödinger equation (see the Appendix for the MATLAB codes of the model). Hence, the theoretical NP energy value of sample M3 could be estimated. The estimated value is 934meV, which is in good agreement with the measured value of $920 \pm 5\text{meV}$, and is consistent with the theoretical value of 923.7meV calculated by the 6+2-band $k \cdot p$ method [73,74]. The parameters used for the calculation are obtained by linear interpolation between the parameters of Si and Ge (as shown in Table 2) [19,75].

For samples D6 and D7, the theoretical calculations of the band structures are more complex, when taking interwell coupling effects in these two samples into

consideration. By employing calculations based on the 6+2-band $k \cdot p$ method, the calculated NP transition energy values of samples D6 and D7 are 908.4meV and 906meV, respectively. These values are in close agreement with the measured value of $907 \pm 3\text{meV}$ and $904 \pm 2\text{meV}$, respectively. The consistency between the measured and theoretical values further confirms that the interwell coupling effect is present in samples D6 and D7. Therefore, intersubband transition, which is the essential phenomenon in QC structures, could be obtained in these samples.

Table 2 Parameters used in the calculations. Note: a_c , a_v and b are obtained from Ref. 19 and other parameters are obtained from Ref. 75.

Parameters	Si	Ge
Lattice constant a_0 (Å)	5.431	5.658
Spin-orbit splitting energy Δ_0 (eV)	0.044	0.296
Optical matrix parameter E_p (eV)	21.6	26.3
Deformation potential constant a_c (eV)	4.88	2.55
Deformation potential constant a_v (eV)	2.46	2.55
Shear deformation potential b (eV)	-2.33	-2.08
Uniaxial deformation potential Ξ_u^d (eV)	9.29	10.20
Elastic constant c_{11} (Mbar)	1.675	1.315
Elastic constant c_{12} (Mbar)	0.65	0.494
Luttinger parameter γ_1	4.22	13.4
Luttinger parameter γ_2	0.39	4.25
Luttinger parameter γ_3	1.44	5.69
Longitudinal mass m_l^* (m_0)	0.9163	0.7991
Transverse mass m_t^* (m_0)	0.1905	0.2

4.5 Samples SL1 and SL2

4.5.1 Experiments

As mentioned in the previous section, the interwell coupling effect, which could lead to the intersubband transitions, was observed in the symmetric DQWs samples D6 and D7. Therefore, in this section, we investigate the active region of the quantum staircase design (introduced in section 2.4) that is the SiGe/Si superlattice structure. In the experiment, two superlattice structures were grown by the UHV-CVD system at substrate temperature of 530°C. Sample SL1 comprises 5 periods of $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_z = 6\text{nm}$)/Si ($L_b = 2\text{nm}$) layers, while sample SL2 comprises 10 periods of $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_z = 6\text{nm}$)/Si ($L_b = 4\text{nm}$) layers. The schematic diagrams and the cross sectional TEM scans of samples SL1 and SL2 are given in Figure 4.20.

Figure 4.20 Schematic diagrams and TEM scans of samples SL1 and SL2

4.5.2 Results and Discussion

High resolution XRD measurements were conducted to analyze the material quality and the compositions of samples SL1 and SL2. The experimental and simulated XRD rocking curves are shown in Figure 4.21. 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. For sample SL1, the simulation was performed based on a 5-period 5.8nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW and 1.9nm-thick Si barrier stack, while the simulation of sample SL2 was performed based on a 10-period 5.7nm-thick $\text{Si}_{0.65}\text{Ge}_{0.35}$ QW and 3.7nm-thick Si barrier stack. There are certain satellite peaks 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 Figure 4.20).

Figure 4.21 Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples SL1 and SL2 (from top to bottom)

Room temperature Fourier transform infrared (FTIR) spectroscopy and low temperature (14K) optical transmission measurements were implemented on samples SL1, SL2 and a Si substrate. For the FTIR measurements, the samples were back polished and the facets of the samples were polished to a 45° inclined plane. The light is injected into the facet of the sample and reflected by the surfaces of the sample, and

then emits from the other facet. The signal was then detected by a liquid N₂ cooled Ge detector. The FTIR spectra of samples SL1, SL2 and the Si substrate are shown in the top portion of Figure 4.22. The intensity difference of the spectra is due to the widths of the samples, which is the distance between the two facets. The bottom portion of Figure 4.22 shows the intensity ratio of the Si substrate to the samples. The ratio is almost constant. It implies that no photon was absorbed by the grown superlattice structures in samples SL1 and SL2. In order to find out whether the temperature of the measurement environment is the reason for the failure of detecting intersubband photoabsorption, a low temperature optical transmission system was set up. The light goes through a chopper and monochromator, and then transit through the sample from the surface. Thereafter, the signal is detected by a liquid N₂ cooled Ge detector. The sample is mounted in a cold finger cooled by compressed helium. Figure 4.23 shows the spectra detected from the optical transmission system. Unfortunately, no intersubband absorption was observed in this experiment either.

Figure 4.22 FTIR spectra of samples SL1, SL2 and a Si substrate (top). Intensity ratio of the Si substrate to the samples (bottom).

Figure 4.23 Optical transmission spectra of samples SL1, SL2 and a Si substrate (top). Intensity ratio of the Si substrate to the samples (bottom)

In summary, intersubband photoabsorption was not resolved in the superlattice samples. This is caused by the poor crystal quality of the samples, which is further proved by the weak PL spectra of the SiGe QWs in these samples (as shown in Figure 4.24). The PL spectrum of sample SL2, which comprises 10 SiGe QWs, is even weaker. This is due to the relatively larger accumulated strain, which causes more interfacial defects.

Figure 4.24 PL spectra of samples SL1 and SL2

4.6 Samples SLD1, SLD2, SLD3 and TQWs

4.6.1 Experiments

In this experiment, four samples (SLD1, SLD2, SLD3 and TQWs) with p-type contact layers were grown by the UHV-CVD system. For sample SLD1, a bottom contact layer (200nm Si layer) was grown before 5-period $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_z = 6\text{nm}$) / Si ($L_b = 2\text{nm}$) superlattice layers. The sample was then capped by a 200nm Si layer (top contact layer). Samples SLD2 and SLD3 have similar structures. Both of the samples comprise 3-stack 5-period $\text{Si}_{0.6}\text{Ge}_{0.4}$ ($L_z = 6, 5\text{nm}$) / Si ($L_b = 2, 3\text{nm}$) superlattice layers. A 100nm Si spacing layer was inserted between every two stacks of the superlattice layers to limit the total strain. The top and bottom contact layers were also included in samples SLD2 and SLD3. Sample TQWs comprises 200nm top and bottom contacts and 3-period triple quantum wells (8nm $\text{Si}_{0.6}\text{Ge}_{0.4}$ /2nm Si/4.5nm $\text{Si}_{0.6}\text{Ge}_{0.4}$ /2nm Si/6nm $\text{Si}_{0.6}\text{Ge}_{0.4}$). A 100nm Si spacing layer was also inserted between every two TQWs stack. All of the contact layers and the centre of the spacing layers were *in situ* doped by boron at 10^{19}cm^{-3} . The schematic diagram and TEM scan of sample SLD2 is shown in Figure 4.25.

Figure 4.25 Schematic diagram and TEM scan of samples SLD2

4.6.2 Results and Discussion

High resolution XRD measurements were implemented on samples SLD1, SLD2 and SLD3. Figure 4.26 shows the experimental and simulated rocking curves of the XRD measurements. For sample SLD1, the simulation was conducted based on a 5-period 5.7nm Si_{0.65}Ge_{0.35} quantum wells and 2nm Si barriers stack. For sample SLD2, the simulation was conducted based on three stacks of 5-period 5.8nm Si_{0.65}Ge_{0.35} quantum wells and 1.8nm Si barriers, while the simulation of sample SLD3 was performed based on three stacks of 5-period 4.6nm Si_{0.66}Ge_{0.34} quantum wells and 2.8nm Si barriers. Comparing the experimental XRD rocking curves with the simulation results, many subordinate satellites were missed. This implies the poor crystal quality of the samples. Figure 4.25 shows the TEM micrograph of a single period SiGe/Si superlattice in sample SLD2, which has quite poor interfaces between the QWs and barriers.

Figure 4.26 Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples SLD1, SLD2 and SLD3 (from top to bottom)

Aluminum ohmic contacts were made on samples SLD1, SLD2, SLD3 and TQWs by E-beam evaporation. The I-V characteristics of these samples were shown in Figure 4.27. Both forward and reverse bias was applied on the samples. The discontinuities at 0V in the I-V curves imply that the devices have different resistance under forward and reverse bias. This is because the doping concentration of the top contact (10^{19}cm^{-3}) is higher than that of the bottom contact ($5\times 10^{16}\text{cm}^{-3}$) in the samples. Therefore, the forward current is larger than the reverse current, when the same amount of bias voltage is applied. However, the intersubband resonant tunneling effect was not resolved in these samples. Thereafter, the optical transmission measurements were implemented on a silicon substrate and the samples without Al ohmic contacts. The transmission spectra and the change of transmission are shown in Figure 4.28. Unfortunately, the intersubband photoabsorption was not observed in these samples.

Figure 4.27 I-V characteristics of samples SLD1, SLD2, SLD3 and TQWs

Figure 4.28 Optical transmission spectra of samples SLD1, SLD2, SLD3, TQWs and a Si substrate (top). Intensity ratio of the Si substrate to the samples (bottom)

In summary, neither resonant tunneling effect nor intersubband photoabsorption was observed in samples SLD1, SLD2, SLD3 and TQWs. The poor material quality could be seen in the TEM scan in Figure 4.25, where rough interfaces of the QWs and

barriers could be observed. The PL spectra of the SiGe QWs in these samples (as shown in Figure 4.29) are very weak and noisy, which further prove the poor crystal quality of the samples.

Figure 4.29 PL spectra of samples SLD1, SLD2, SLD3 and TQWs

In conclusion, the intersubband transitions of the SiGe/Si superlattice structures were not obtained from either undoped (samples SL1 and SL2) or doped samples (samples SLD1, SLD2, SLD3 and TQWs). As stated, the reason for the failure is the poor material quality, which is mainly induced by the high growth rate of the SiGe epilayers (12.8nm/min). In order to grow the quantum cascade structures with very thin epilayers (as thin as 1nm), the growth rate of the SiGe epilayers must be reduced to 1nm/min or lower. Unfortunately, there is not much room for further reduction due to the constraint of our UHV-CVD system. However, it is good to learn the implementation of the UHV-CVD system for growing the SiGe/Si QC structure.

Chapter 5 Conclusion and Recommendations

5.1 Conclusion

In this thesis, I have studied the SiGe/Si heterostructures, which are discussed on development of a SiGe/Si quantum cascade structure in the purpose of fabricating a QCE. The research in the past two years was related to a wide range, and it primarily consisted of the theoretical background, device design and fabrication of the SiGe/Si quantum cascade structures, further more, experimental testing and characterization of the various structures.

First, a SiGe/Si quantum cascade emitter was grown by the UHV-CVD system in IME, and fabricated structure is similar to the quantum staircase emitter described in reference 43. However, no EL or PL signal was observed from this sample. It is probably due to the poor quality in the relaxed buffer layer. In our present epitaxial system, it is difficult to grow very thin epilayers. The limitation of our epitaxial system may also have contributed to the poor performance of the fabricated device.

Thereafter, samples with MQWs structures (M1, M2 and M3) have tried to grow to investigate the QW characteristics. The quantum confinement effect is supposed to be observed in these samples because of the different width for each QW. However, only PL signals of samples M2 and M3 were detected, and the confinement effect of these

two samples is not so strong. The annealing effect was also studied on these samples. Since a rapid thermal annealing can result on a clear reduction of the defect density in the SiGe/Si heterostructures, the PL intensity of the annealed samples has been enhanced and the energy shifts between the NP and TO peaks of the three samples are clearly observed.

After studying on the MQWs, DQWs structures were grown to investigate the interwell coupling effect. PL measurements were carried out on the asymmetrical DQWs (samples D1, D2, D3, D4 and D5) and the symmetrical DQWs (samples D6 and D7). The PL spectra of the five asymmetrical samples show a certain coupling effect. The PL intensity of the narrow well decreases as the barrier thickness decreases. It shows that a thinner barrier enhances the tunneling effect between the two QWs. For the symmetrical DQWs, the interwell coupling effect is observed. There is a 16meV energy difference between the NP peaks of samples D6 and M3, which is considered as a single QW due to its thick barrier.

Finally, the SiGe/Si superlattice structures, which are the active regions of quantum staircase structures, were investigated. Both undoped (samples SL1 and SL2) and doped (samples SLD1, SLD2, SLD3 and TQWs) samples were prepared. The FTIR, optical transmission and I-V characteristics were performed for these samples. No intersubband transitions were observed. It comes from a poor crystal quality of the samples, which is verified by the TEM and PL spectroscopy.

5.2 Recommendations for Future Work

As stated in the previous section, the intersubband transitions of the SiGe/Si quantum cascade structures were not obtained in this project. This is mainly caused by the poor material quality, which is gravely affected by the high growth rate of the $\text{Si}_{0.6}\text{Ge}_{0.4}$ epilayers (12.8nm/min). Therefore, I suggest using MBE to grow the SiGe/Si QC structures. This is because MBE could achieve relatively better interfaces between the barriers and QWs, and lower growth rate.

Another way to improve the material quality is to reduce the growth rate of the SiGe epilayers. Hence, finer SiGe QWs could be obtained. According to the growth rate equations in section 3.1.3, reducing the growth temperature and the flow rate of the source gases could lead to a lower growth rate. However, the temperature used in our experiment to grow the $\text{Si}_{0.6}\text{Ge}_{0.4}$ QWs is 530°C. There is not much room for further reduction, because the H (hydrogen) terminated SiGe surface will start to form when the growth temperature is lower than 500°C [76]. Reducing the flow rate of the source gases is also difficult. The flow rate of Si_2H_6 used in our growth is only 5sccm. It is not possible to further reduce this flow rate in our system. Mixing Si_2H_6 with other gas (such as argon) is a practical way to reduce the total flow rate of the source gas. However, this requires modifying the installations of the source gases control system.

Besides the quantum staircase design which uses the SiGe/Si superlattice as the active

region, the quantum cascade structure using triple quantum wells as the active region is a potential structure. The electroluminescence from this kind of design by using GaAs/AlGaAs material system has been demonstrated already [77]. In addition, the intersubband photoluminescence study on the quantum cascade structure using either the SiGe/Si superlattice or the triple quantum wells as the active region would be very interesting, and it is more straightforward than the far-infrared photoabsorption studies.

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Author's Publication

Interwell coupling effect in Si/SiGe quantum wells grown by ultra high vacuum chemical vapor deposition

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Abstract Si/Si_{0.66}Ge_{0.34} coupled quantum well (CQW) structures with different barrier thickness of 40, 4 and 2 nm were grown on Si substrates using an ultra high vacuum chemical vapor deposition (UHV-CVD) system. The samples were characterized using high resolution x-ray diffraction (HRXRD), cross-sectional transmission electron microscopy (XTEM) and photoluminescence (PL) spectroscopy. Blue shift in PL peak energy due to interwell coupling was observed in the CQWs following increase in the Si barrier thickness. The Si/SiGe heterostructure growth process and theoretical band structure model was validated by comparing the energy of the no-phonon peak calculated by the 6 + 2-band *k*·*p* method with experimental PL data. Close agreement between theoretical calculations and experimental data was obtained.

Keywords Si/SiGe · Coupled quantum well · UHV-CVD

Introduction

Silicon is notably the most widely used semiconductor in the microelectronics industry. As such, the ability to

realize light emitters based on silicon is a highly desirable goal that could lead to integrating optical and microelectronic functions on the same silicon-based platform. However, the indirect band characteristic of silicon prohibits the efficient radiative recombination of electrons and holes to result in coherent optical emission. Currently, there are a number of efforts to overcome this physical challenge, such as the use of Si nanocrystals and Er coupled Si [1–3]. Apart from these potential solutions, the quantum cascade (QC) structure is considered a promising method to realize a Si-based coherent light emitter. This is because the carrier transition mechanism for the QC structure is based on intersubband transition. Hence, the indirect band property of Si and SiGe alloy could be ignored.

Recently, intersubband photoluminescence (PL) and electroluminescence (EL) have been demonstrated in Si/SiGe QC structures [4–6]. Compared with other solutions, the emission wavelength of the QC emitter (QCE) lies at the mid- to far-infrared (also called terahertz) region, which is currently under utilized due to the lack of suitable material systems. In the QC structure, the active region is normally formed by the Si/SiGe superlattice layers, which comprise several layers of SiGe quantum wells (QWs) and Si barriers. In such a structure, interwell coupling effect plays an essential role to determine the energy transitions and resultant optical and electronic properties of the Si/SiGe QC structure. In other words, the intersubband transitions in the QC structures rely on the interwell coupling in the QWs. This is because the wave functions in the QC structures are no longer confined to a single well, but penetrate into barriers and extend over the entire region [7]. Therefore, the study of interwell coupling effect in the QWs remains a critical issue for

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realizing the QCE. Luminescence from CQWs in Si/SiGe materials grown by molecular beam epitaxy (MBE) has been reported by Fukatsu et al. [8–10]. However, in their reports, the Ge fraction in the SiGe QWs is less than 20%. This is not suitable for application in the QC structures, because the resulting valence band offset is only about 0.1 eV.

In this paper, we present a photoluminescence (PL) study on strained Si/Si_{0.66}Ge_{0.34} CQWs grown by ultra high vacuum chemical vapor deposition (UHV-CVD). The Ge fraction in our SiGe QW samples is about twice the Ge fraction in the samples reported by Fukatsu et al. [8–10]. The higher Ge fraction in our samples is expected to produce an effectively larger valence band offset, which is more appropriate for design of the QC structure for light emission. The interwell coupling effect in the QC samples of different barrier thickness was investigated. Comparison with theoretical calculation of the energy transitions is presented.

Experimental details

The samples used in this study were grown in a UHV-CVD cold-wall 8-inch single-wafer epitaxy reactor. The chamber pressure is below 10^{-9} Pa. The reactant gases used for the deposition are disilane (Si₂H₆) and germane (GeH₄). P-type (boron doped at $2.5 \times 10^{15} \text{ cm}^{-3}$) Si (100) substrates were cleaned using a standard solution comprising 10DI:2H₂O₂:1NH₄OH (by volume), then dipped into dilute HF (DHF) solution comprising 200H₂O:1HF for 2 min before deposition. Figure 1 shows the schematic diagrams of the structures and growth conditions of the three samples investigated in this study. A 3 nm-thick Si buffer layer was grown at 530°C at 1 nm/min on the p-type silicon substrate. This is followed by growth of the SiGe QWs, Si barriers and the Si cap layer. The SiGe QWs in sample 1 was deposited at 530°C at growth rate of 12 nm/min, while the Si barrier and cap layer were deposited at 600°C at 10 nm/min. In samples 2 and 3, the thin Si barriers between the two CQWs (4 nm and 2 nm, respectively) were grown under the same condition as the 3 nm-thick Si buffer layer. The thick Si barriers in sample 3 and the QWs and cap layers in both samples 2 and 3 were grown under the same condition as the barriers, the QWs and cap layer of sample 1, respectively. All the layers are nominally undoped.

Photoluminescence (PL) measurements were carried out at 4 K by exciting the sample using the 514.5 nm line from an Ar ion laser. The PL was detected by a

Fig. 1 Schematic diagrams of structures and growth conditions of samples 1, 2 and 3 used in this study. The samples are grown by UHV-CVD. Note: T_s and GR refers to substrate temperature and growth rate, respectively

liquid nitrogen cooled Ge detector in conjunction with a standard lock-in technique. The structural characteristic of the samples, such as interface roughness, layer thickness and Ge concentration were characterized using cross-sectional transmission electron microscopy (XTEM) and high resolution x-ray diffraction (HRXRD).

Results and discussion

Figure 2 shows the x-ray rocking curves of samples 1–3. The sharp peaks 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. For sample 1, the simulation was performed based on a 10-period

5.7 nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW and 40 nm-thick Si barrier stack. For sample 2, the simulation was performed based on a 5.7 nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW, 4 nm-thick Si barrier and 5.7 nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW. Finally for sample 3, the simulation was performed based on a 5-period 5.6 nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW, 2 nm-thick Si barrier, and 5.6 nm-thick $\text{Si}_{0.66}\text{Ge}_{0.34}$ QW and 40 nm-thick Si barrier stack. As shown in the figure, 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 are confirmed by XTEM examination of the samples as shown in Fig. 3. The dark regions correspond to the SiGe QWs, while the relatively bright regions correspond to the Si barriers. The XTEM micrographs show that the high degree of strain (up to 1.5%) between the QWs and barriers gave rise to substantial thickness variations (the roughness is about 7 Å) in the QWs and barriers.

The thickness variations in the QWs and barriers result in the relatively weak and broad PL spectra of the SiGe QWs observed in samples 1–3, as shown in Fig. 4. In the figure, NP, TA and TO refers to no-phonon, transverse-acoustic phonon-assisted and transverse-optical phonon-assisted transitions, respectively [11]. The full-width at half maximum (FWHM) of the PL signal of sample 1 is about 40 meV (as marked in Fig. 4). The contribution to the FWHM of this signal by interface roughness (ΔL) could be estimated by the following equations [12, 13]:

$$\Delta E = \left[\frac{dE_{1e}}{dL} + \frac{dE_{1hh}}{dL} \right] \Delta L \quad (1)$$

$$\frac{dE_{1e}}{dL} = \frac{E_{1e}}{\frac{L}{2} + \frac{\hbar}{\sqrt{2m_e^B(\Delta E_c - E_{1e})}} \cos^2 \left(\frac{L}{2} \sqrt{\frac{2m_e^W E_{1e}}{\hbar^2}} \right) + \frac{\hbar}{\sqrt{8m_e^W E_{1e}}} \sin \left(L \sqrt{\frac{2m_e^W E_{1e}}{\hbar^2}} \right)} \quad (2)$$

$$\frac{dE_{1hh}}{dL} = \frac{E_{1hh}}{\frac{L}{2} + \frac{\hbar}{\sqrt{2m_{hh}^B(\Delta E_v - E_{1hh})}} \cos^2 \left(\frac{L}{2} \sqrt{\frac{2m_{hh}^W E_{1hh}}{\hbar^2}} \right) + \frac{\hbar}{\sqrt{8m_{hh}^W E_{1hh}}} \sin \left(L \sqrt{\frac{2m_{hh}^W E_{1hh}}{\hbar^2}} \right)} \quad (3)$$

where L is the QW width and E_{1e} and E_{1hh} are the energy values of the first energy state in the conduction and valence bands. m_e^B , m_e^W , m_{hh}^B and m_{hh}^W are the effective mass of the electron and heavy hole in the QW

(W) and barrier (B), and ΔE_c and ΔE_v are the band offsets of the conduction and valence bands, respectively. Hence, out of the total FWHM of 40 meV, 13.1 meV is contributed by the interface roughness between the QW and barrier layers. The large difference of ~27 meV between the estimated and measured FWHM values could be due to the presence of interface defects, which are caused by the partial strain relaxation due to lattice mismatch at the interface.

In Fig. 4, the PL peaks shift to lower energy following decrease in the barrier thickness. This is due to the effect of interwell coupling between the two symmetrically-aligned wells caused by the wavefunction penetration across the Si barrier. When two quantum wells are brought close enough, such as the case of samples 2 and 3, the energy states in both the conduction and valence bands are split into symmetric (S) and anti-symmetric (A) states due to the coupling effect (as shown in the inset of Fig. 4). In the valence band, both the heavy hole (HH) and light hole (LH) states are split. However, the energy of the HH S-state is higher than that of the LH S-state (the difference is about 60 meV in our calculation). Hence, the observed luminescence should be attributed to the optical transition between the S-states of electrons and the HH states in the valence band. The energy of HH S-state is higher than that of the HH state before split (the difference is about 15 meV in our calculation). Therefore the NP transition energy reduces in the presence of coupling effect. This explains the observation that red shift of the PL peak energy follows a reduction in barrier thickness. Note that the band energy changes in the conduction band could be ignored, because the band offsets in the conduction bands in our samples are very small.

In sample 1, since the thickness of the Si barrier is 40 nm, the QWs in this sample should be effectively isolated from each other. This being the case, it should have similar characteristic as a single QW (SQW) with

Fig. 2 Experimental and simulated x-ray rocking curves of the symmetric (0 0 4) reflection for samples 1, 2 and 3 (from top to bottom)

the same QW width and Ge composition. The band structure of a strained $\text{Si}_{0.66}\text{Ge}_{0.34}$ SQW grown on Si substrate is shown in Fig. 5. For a strained $\text{Si}_{1-x}\text{Ge}_x$ layer ($x < 0.4$) grown on Si substrate, the indirect bandgap E_g at 4.2 K can be expressed as [14]:

$$E_{g,\text{SiGe}}(x) = 1.17 - 0.896x + 0.396x^2 \text{ (eV)} \quad (4)$$

The valence band discontinuity is given by the following equation [15]:

$$\Delta E_v = 0.74x \text{ (eV)} \quad (5)$$

Fig. 3 XTEM micrographs of (a) sample 1, (b) sample 2 and (c) sample 3. Dark and bright regions correspond to the SiGe QW and Si barrier layers, respectively

Hence the conduction band offset could be obtained by:

$$\Delta E_c = -0.156x + 0.396x^2 \quad (6)$$

If the value of ΔE_c is positive, the band alignment is type-II, otherwise the band alignment is type-I.

Fig. 4 PL spectra of samples 1, 2 and 3 (from bottom to top) measured at 4.2 K. The barrier thickness (L_b) of samples 1, 2 and 3 are 40, 4 and 2 nm, respectively. Inset shows the band structure of the CQWs. S and A represent the symmetric and anti-symmetric states, respectively [9]

Fig. 5 Schematic diagram of the band structure of a strained $\text{Si}_{0.66}\text{Ge}_{0.34}$ layer grown on Si substrate. Note: E_g is the bandgap, E_c , E_v , is the conduction and valence band, respectively, and ΔE_c , ΔE_v is the conduction band and valence band discontinuities, respectively. The values of the energies shown in the figure are calculated at 4.2 K

According to the work of Van de Walle and Martin [15, 16], the energy splitting of the valence band is given by the following equations:

$$\Delta E_{v,1} = -\frac{1}{6}\Delta_0 + \frac{1}{4}\delta E + \frac{1}{2}\left[\Delta_0^2 + \Delta_0\delta E + \frac{9}{4}(\delta E)^2\right]^{1/2} \quad (7)$$

$$\Delta E_{v,2} = \frac{1}{3}\Delta_0 - \frac{1}{2}\delta E \quad (8)$$

$$\Delta E_{v,3} = -\frac{1}{6}\Delta_0 + \frac{1}{4}\delta E - \frac{1}{2}\left[\Delta_0^2 + \Delta_0\delta E + \frac{9}{4}(\delta E)^2\right]^{1/2} \quad (9)$$

where Δ_0 is the spin-orbital splitting. For strain along the (001) direction, δE is equal to $2b(\epsilon_{\perp} - \epsilon_{\parallel})$, where b

is the uniaxial deformation potential for tetragonal strain. $\Delta E_{v,1}$, $\Delta E_{v,2}$ and $\Delta E_{v,3}$ represent the band energy offsets of the light, heavy and split-off band at the valence band, respectively. The energy splitting of the conduction band is given by the following equations:

$$\Delta E_c^{001} = \frac{2}{3}\Xi_u^{\Delta}(\epsilon_{\perp} - \epsilon_{\parallel}) \quad (10)$$

$$\Delta E_c^{100,010} = -\frac{1}{3}\Xi_u^{\Delta}(\epsilon_{\perp} - \epsilon_{\parallel}) \quad (11)$$

where Ξ_u^{Δ} is the uniaxial strain deformation potential for the conduction band. Hence, the theoretical NP energy value of sample 1 could be estimated by the above equations. The estimated value is 934 meV, which is in good agreement with the measured value of 920 ± 5 meV, and is consistent with the theoretical value of 923.7 meV calculated by the 6 + 2-band $k \cdot p$ method. The parameters used for the calculation are obtained by linear interpolation between the parameters of Si and Ge (as shown in Table 1) [17, 18].

For samples 2 and 3, the theoretical calculations of the band structures are more complex, when taking interwell coupling effects in these two samples into consideration. By employing calculations based on the 6 + 2-band $k \cdot p$ method [19, 20], the calculated NP transition energy values of samples 2 and 3 are 908.4 meV and 906 meV, respectively. These values are in close agreement with the measured value of 907 ± 3 meV and 904 ± 2 meV, respectively. The consistency between the measured and theoretical values further confirms that the interwell coupling effect is present in samples 2 and 3. Therefore, inter-subband transition, which is the essential phenomenon

Table 1 Parameters used in the calculations. Note: a_c , a_v and b are obtained from Ref. 15 and other parameters are obtained from Ref. 18

Parameters	Si	Ge
Lattice constant a_0 (Å)	5.431	5.658
Spin-orbit splitting energy Δ_0 (eV)	0.044	0.296
Optical matrix parameter E_p (eV)	21.6	26.3
Deformation potential constant a_c (eV)	4.88	2.55
Deformation potential constant a_v (eV)	2.46	2.55
Shear deformation potential b (eV)	-2.33	-2.08
Uniaxial deformation potential Ξ_u^{Δ} (eV)	9.29	10.20
Elastic constant c_{11} (Mbar)	1.675	1.315
Elastic constant c_{12} (Mbar)	0.65	0.494
Luttinger parameter γ_1	4.22	13.4
Luttinger parameter γ_2	0.39	4.25
Luttinger parameter γ_3	1.44	5.69
Longitudinal mass m_l^* (m_0)	0.9163	0.7991
Transverse mass m_t^* (m_0)	0.1905	0.2

in QC emitters, could be obtained in these samples. This will be verified in the future experiments.

Conclusions

In summary, the interwell coupling effect in Si/Si_{0.66}Ge_{0.34} CQWs structures grown by UHV-CVD was investigated using low temperature PL measurements. Red shift of PL peak energy caused by interwell coupling was observed following a reduction in barrier thickness. Variations in the QW and barrier thickness and possibly defects in the as-grown material could have contributed to the relatively broad PL signals from the samples. The band structure model of the Si/SiGe heterostructure was validated by comparing theoretical calculations based on the 6 + 2-band $k \cdot p$ method with experimental values of the no-phonon PL peak. The close agreement between the measured data and theoretical calculations confirms the presence of the interwell coupling effect in samples with narrow barriers. The results from this work are useful for future growth and design of Si/SiGe QC emitters.

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Band structure investigation of strained $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ coupled quantum wells

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Abstract: The band structure of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ coupled quantum wells (CQW) was calculated with the 8-band $k \cdot p$ method. Both strain and spin-orbit split-off band effect were taken into account. The subband energy of the $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ quantum well as a function of barrier width and well width was calculated. Barrier width varies between 20–60 Å while well width varies between 30–110 Å. Finally, the relationship between subband energy and Ge composition range from 10% to 60% was also shown.

Keywords: band structure; coupled quantum well; 8-band $k \cdot p$ method; strain effect; valence band; hole subband energy; coupling effect.

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1 Introduction

During the past two decades, $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ structures have attracted more and more attention. The transitions in single quantum well (SQW) have already been calculated and demonstrated by many researchers. The broadband absorption of 8.1 μm and 8–14 μm with SQW structure were reported long ago [1,2]. Also, Fukatsu and Shiraki [3] reported the photoluminescence from strained SiGe/Si coupled double quantum well (CDQW) systems. The realisation of the quantum cascade laser (QCL) [4] initiated strong interest in developing a SiGe based laser. Dehlinger et al. [5] reported the intersubband transition electroluminescence between the first two heavy hole energy states (HH1–HH2) from silicon-based quantum cascade structures. The extremely long strain balanced Si/SiGe structure was demonstrated by another research group and terahertz electroluminescence between the first heavy/light hole states (HH1–LH1) was observed [6]. Though the lack of a real Si-based laser is still a challenge to all researchers [7]. The possible solution is to make use of the QCL fundamentals due to the indirect band gap property of Si. However, among most quantum cascade structures designed, the active region contains more than one quantum well with thin barriers. The wave functions are no longer confined to a single well but penetrate into barriers and extend over the whole region [4], which results in an interaction between energy states in nearby quantum wells called coupling. Therefore the study of interwell interacting effects is a critical issue. The purpose of our investigation is to show a detailed procedure for calculating the valence band confined energy levels in strained $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ CQWs. As a result, as a function of barrier width L_b , Ge concentration x and well width L_z , the valence band structures are calculated with the 8-band $k \cdot p$ method, at $k = 0$ band edge.

2 Calculation method

The CQW structure is assumed to be grown on an Si (001) oriented substrate. The CQW profile we investigated is shown in Figure 1(a). The coupled well widths are represented by L_{z1} and L_{z2} , respectively, and L_b is the Si barrier layer width. One period of the CQW is taken as $L = L_{z1} + L_{z2} + 2L_b$, with origin $z = 0$ located at the centre of L_{z1} . The band structure of the CQWs was calculated with the 8-band $k \cdot p$ model including first conduction band, heavy hole, light hole and spin-orbit splitting bands. The strain effect was also taken into account [8,9]. The $\sim 4.2\%$ mismatch between Si and Ge lattices induces the in-plane strain $\varepsilon_{\parallel}$ perpendicular to the growth direction and the shear strain $\varepsilon_{\perp}$ along the growth direction [9], which are represented by

$$\varepsilon_{\parallel} = \varepsilon_{xx} = \varepsilon_{yy} = \frac{a_{\text{Si}} - a_{\text{Si}_{1-x}\text{Ge}_x}}{a_{\text{Si}_{1-x}\text{Ge}_x}} \quad (1)$$

$$\varepsilon_{\perp} = \varepsilon_{zz} = -2 \frac{C_{12}}{C_{11}} \varepsilon_{\parallel}, \quad (2)$$

where a_{Si} and $a_{\text{Si}_{1-x}\text{Ge}_x}$ are the lattice constants of barrier material (Si) and the well material ($\text{Si}_{1-x}\text{Ge}_x$). C_{11} and C_{12} are the elastic stiffness constants. The energy shifts due to strain are defined respectively as [9]

$$\delta E_{hy} = 2(a_c - a_v)(1 - c_{12}/c_{11})\varepsilon_{\parallel} \quad (3)$$

$$Q_e = -b(1 + 2c_{12}/c_{11})\varepsilon_{\parallel}, \quad (4)$$

where δE_{hy} and Q_e are the hydrostatic and shear deformation energies, a_c , a_v and b are the deformation potential constants. The total Hamiltonian including strain effect to be solved is given by [8]

$$H = H_K + H_S + V_{(z)}. \quad (5)$$

The wave function is written as [10]

$$\Psi_{k_z(z)} = \sum_{i=1}^8 e^{ik_{\parallel} r_i} \phi_{i(z)} u_{i(r)}, \quad (6)$$

where $k = k_x \bar{i} + k_y \bar{j}$, $r = x\bar{i} + y\bar{j}$, $r = x\bar{i} + y\bar{j} + z\bar{k}$, ϕ_i is the envelope function and u_i is the periodic Bloch wave function. Equations (1)–(4) are used to calculate strain related parameters while equations (5) and (6) are used to calculate band edge energy levels. The probability functions $\sum_i P_i^j = 1, (i = e, hh, lh, so)$ [8,10] are also calculated to identify the conduction (*e*), heavy hole (*hh*), light hole (*lh*) and spin-orbit split-off (*so*) band components in the CQW energy states.

Figure 1 Schematic diagram of (a) Coupled Quantum Well and (b) Single Quantum Well

3 Results and discussions

Firstly, to clarify the reliability of our method, the neighbouring well width, L_{z2} is set to zero as shown in Figure 1(b). The structure becomes a SQW structure with barrier width L_b , well width L_{z1} and period $L = L_b + L_{z1}$. 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. [2], $hh1 = 43$, $hh2 = 156$, $lh1 = 91$, $lh2 = 205$, $so1 = 192$ meV, and ones reported by Kahan et al. [11], $hh1 = 42$, $hh2 = 155$, $lh1 = 96$, $lh2 = 199$ and $so1 = 215$ meV.

Figure 2 shows the comparison between the in-plane dispersion curves of the valence hole subbands confined in the CQW and SQW. By comparison, the coupling effect in the CQW can be identified by the energy state changes, as well as the nonparabolic dispersions. Figure 3 shows the corresponding wave functions at $k = 0$ as in Figure 2. Following Figure 1(a), the well widths are $L_{z1} = 50$ Å and $L_{z2} = 100$ Å respectively. The solid line and dashed line show the band structure of QW L_{z1} with different barrier width $L_b = 20/60$ Å. The dispersion curves of $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ (50/200 Å) SQW are also plotted in dotted line. The used parameters are listed in Table 1. Energy states are identified by wave functions and the components of hh , lh and so [10,12], as shown in Table 2. 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. [13] and explains the nonparabolic dispersion relations at higher k . Another significance of CQW is the energy state shift. As shown in Figure 2, 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 Figure 3). Both of CQW and SQW energy levels hh , lh and so were calculated with the mentioned 8-band $k \cdot p$ model.

Figure 2 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 $L_b = 20/60$ Å. While the dotted line shows the dispersion curves of $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ (50/200 Å) 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

Figure 3 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

Table 1 Parameters used in the band structure calculations. All parameters are obtained from [14]. Linear interpolation is taken and band offset $\Delta E_v = 0.84x \text{ eV}$ [15]

	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} (MPa)	1.675	1.315
Stiffness C_{12} (MPa)	0.65	0.494

Table 2 Components of hh , lh and so in valence subbands in $\text{Si}_{0.6}\text{Ge}_{0.4}/\text{Si}$ CQW and SQW

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%

Figure 4 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 to -0.1 meV and -1.3 meV, respectively, when L_b is increased from $20 \text{ \AA}$ to $60 \text{ \AA}$. On the other hand, the $lh1$ state has an energy change of 13.3 meV. From Table 2 and Figure 3 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 Figure 2.).

Figure 4 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 $50 \text{ \AA}$ and $100 \text{ \AA}$

Figure 5 shows the energy dependence as a function of well width L_{z1} . The barrier width L_b is fixed at $30 \text{ \AA}$ and $L_{z2} = 100 \text{ \AA}$. As L_{z1} is increased from $30 \text{ \AA}$ to $110 \text{ \AA}$, all the three energy levels increase, but an intersection happens at $L_{z1} = 46 \text{ \AA}$ between $hh2$ and $lh1$. From Figure 5 we also find hh states increase faster than lh state at $L_{z1} < 110 \text{ \AA}$. Since the barrier width is $30 \text{ \AA}$, interwell coupling is to be taken into account. Whereas, as shown in Figure 2, 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 5 Energy dependence as a function of well width L_{z1}

Figure 6 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 $\Delta E_v = 0.84x$, [15] the zero energy reference changes with changing x , therefore we use the top valence band edge of barrier (Si) as new zero reference to normalise 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 $Si_{1-x}Ge_x$.

Figure 6 Energy dependence as a function of Ge composition in well material

4 Conclusion

The valence band structure of $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ CQW was calculated. The strain dependent energies are derived with an 8-band $k \cdot p$ method, with spin-orbit interaction effects being taken into account. At $k = 0$ point, it was found that the interwell coupling has more effect on higher energy hole states, such as $lh1$. The dependence of hole energy on barrier width, well width and Ge composition was also calculated, which provides a good reference for intersubband transition designs with $\text{Si}_{1-x}\text{Ge}_x/\text{Si}$ structures.

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440 F. Lu et al.

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Appendix

```
%sel=0, calculate HH with plot; sel=2, calculate HH without plot.
%sel=1, calculate LH with plot; sel=3, calculate LH without plot.
%x is the Ge composition of QW, y is the Ge composition of VS.
%L is the width of QW in nm.
function [E] = energy (sel,x,y,L)
global hbar R mw mb j Lw;

hbar=1.05457e-34;
Lw=L.*1e-9;
sel0=sel;

%Luttinger parameters.
r1Si=4.22;
r2Si=0.39;
r1Ge=13.4;
r2Ge=4.25;
r1w=r1Si+(r1Ge-r1Si).*x;
r2w=r2Si+(r2Ge-r2Si).*x;

%Elastic constants c11 and c12, which are used to calculate constant D.
c11Si=16.577;
c12Si=6.393;
c11Ge=12.853;
c12Ge=4.826;
c11x=c11Si+x.*(c11Ge-c11Si);
c12x=c12Si+x.*(c12Ge-c12Si);

%D will be used to calculate lattice constants perpendicular to the plane.
DSi=2.*(c12Si./c11Si);
Dx=2.*(c12x./c11x);

%Lattice constants of Si and Ge.
aSi=5.43;
aGe=5.65;

ay=aSi.*(1-y)+aGe.*y-0.0188.*y.*(1-y); %Lattice constant of VS
eSi=ay./aSi-1; %Strain of Si barrier in the plane
aSi_p=aSi.*(1-DSi.*eSi); %Lattice constant of Si perpendicular to the
plane
eSi_p=aSi_p./aSi-1; %Strain of Si barrier perpendicular to the
plane
ax=aSi.*(1-x)+aGe.*x-0.0188.*x.*(1-x); %Lattice constant of QW in the plane
ex=ay./ax-1; %Strain of QW in the plane
ax_p=ax.*(1-Dx.*ex); %Lattice constant of QW perpendicular to the
plane
ex_p=ax_p./ax-1; %Strain of Si barrier perpendicular to the
plane

fprintf('\nStrain of Si barrier in the plane is %f\nStrain of Si barrier
perpendicular to the plane is %f\n', eSi,eSi_p)
fprintf('\nStrain of QW in the plane is %f\nStrain of QW perpendicular to the plane
is %f\n', ex,ex_p)

%Calculation of b and delta 0.
bSi=-2.35;
bGe=-2.55;
bx=bSi+x.*(bGe-bSi);
del0Si=0.044;
del0Ge=0.296;
del0x=del0Si+x.*(del0Ge-del0Si);

%delta E of QW and barrier
delEx=2.*bx.*(ex_p-ex);
```

```

delESi=2.*bsi.*(esi_p-esi);

%LH and HH shift from the band edge in terms of the deformation potentials
ElhSi=-1./6.*del0Si+0.25.*delESi+0.5.*sqrt(del0Si.^2+del0Si.*delESi+9./4.*delESi.^2);
;
EhSi=1./3.*del0Si-0.5.*delESi;
fprintf('\nLH edge in Si is %f\nHH edge in Si is %f\n', ElhSi,EhSi)

ElhX=-1./6.*del0x+0.25.*delEx+0.5.*sqrt(del0x.^2+del0x.*delEx+9./4.*delEx.^2);
EhX=1./3.*del0x-0.5.*delEx;
fprintf('LH edge in QW is %f\nHH edge in QW is %f\n\n', ElhX,EhX)

%avSi=2.46;
%avGe=1.24;
%avx=avSi+x.*(avGe-avSi);
%EvavSi=avSi.*(2.*esi+esi_p);
%Evavx =avx.*(2.*ex+ex_p);

Ewav=(0.47-0.06.*y).*(x-y); %Mass average valence band offset between QW and VS.
Ebav=(0.47-0.06.*y).*(0-y); %Mass average valence band offset between barrier and VS.

while (sel>=0)
%Selection of LH and HH
if (sel==0)
    mw=1./(r1w-2.*r2w).*9.1e-31; %HH mass of QW
    mb=1./(r1Si-2.*r2Si).*9.1e-31; %HH mass of barrier
    V0=Ewav-Ebav+EhX-EhSi; %HH band edge offset between barrier and QW.
    fprintf('HH band offset is %f\n',V0)

%Equation of valence band offset from DJ Paul
    Ew=(0.74-0.06.*y).*(x-y);
    Eb=(0.74-0.06.*y).*(0-y);
    Ediff=Ew-Eb; %This value should be comparable with V0h.
    fprintf('Paul''s HH band offset is %f\n', Ediff)

else
    mw=1./(r1w+2.*r2w).*9.1e-31; %LH mass of QW
    mb=1./(r1Si+2.*r2Si).*9.1e-31; %LH mass of barrier
    V0=Ewav-Ebav+ElhX-ElhSi; %LH band edge offset between barrier and QW.
    fprintf('LH band offset is %f\n',V0)
end

%Calculation
R=Lw./2./hbar.*sqrt(2.*mw.*V0.*1.6e-19);
fprintf('The Radius is %f\n\n', R)
i=0;
while(i<=R.*2./pi) %No. of bound states
    j=(-1).^i;
    x1=i.*pi./2;
    x2=(i+1).*pi./2;
    x0=(x1+x2)./2;
    k=yR(x0)-yT(x0);
    while(abs(k)>1e-5) %Accuracy is 0.00001
        if(k>0)
            x1=x0;
            x0=(x0+x2)./2;
        else
            x2=x0;
            x0=(x0+x1)./2;
        end
        k=yR(x0)-yT(x0);
    end
    i=i+1;
end

```

```

i=i+1;
if(sel==0)
    E=En(x0);
    fprintf('HH%d ~ %f\n', i,E)
else
    E=En(x0)+Ehhx-Elhx;
    fprintf('LH%d ~ %f\n', i,E)
end
end
if (sel==2)
    sel=sel-2;
    fprintf('\n')
else
    sel=-1;
end
end
fprintf('\n\n')

%Plot graph
if (sel0==0|sel0==1)
    x1=0:0.00001:R;
    y1=sqrt(R.^2-x1.^2);
    hold off;
    plot (x1,y1)
    hold;

    y1= sqrt(mb./mw).*x1.*tan(x1); %even solution
    plot (x1,y1)

    y1=-sqrt(mb./mw).*x1.*cot(x1); %odd solution
    plot (x1,y1)

    axis([0 R 0 R]);
end

%Subfuntions of calculation part
function [YR] = yR(xr)
global R;
YR=sqrt(R.^2-xr.^2);

function [YT] = yT(xt)
global j mb mw;
if (j==1)
    YT= sqrt(mb./mw).*xt.*tan(xt);
else
    YT=-sqrt(mb./mw).*xt.*cot(xt);
end

function [E]= En(x)
global hbar mw Lw;
k=2.*x./Lw;
E=k.^2.*hbar.^2./2./mw./1.6e-19;

```