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13. ABSTRACT *(Maximum 200 words)*

The purpose of the research was to perform scientific study and experimentation on potential new Si-based devices for future optical and electronic applications. The research areas included novel detectors, sources, new properties, and other quantum devices using Si molecular beam epitaxy (Si-MBE) based superlattices and superstructures. With the current ARO support, we have made significant advances in the understanding of optical properties of intersubband transition of SiGe/Si multiple quantum wells, and the fabrication of multiple quantum well infrared detectors operating in the mid infrared range. Large many-body effects have been observed in heavily doped Si and SiGe/Si quantum well structures. Normal incidence intersubband transitions have been demonstrated for both n and p type SiGe/Si quantum well structures. For potential realization of Si-based light sources we have studied the luminescence from monolayer superlattices and strained alloy layers. In the area of quantum transport, a resonant tunneling transistor has been demonstrated.

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QUANTUM DEVICES USING SI-BASED SUPERLATTICES AND SUPERSTRUCTURES

FINAL TECHNICAL REPORT

KANG L. WANG AND GAMANI KARUNASIRI

FOR THE PERIOD

SEPTEMBER 15, 1989 THROUGH OCTOBER 14, 1992

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1 Statement of the Problem Studied

The purpose of the research was to perform scientific study and experimentation on potential new Si based devices for future optical and electronic applications. The research areas included novel detectors, sources, new properties, and other quantum devices using Si molecular beam epitaxy (Si-MBE) based superlattices and superstructures. The superstructure devices consists of for example, heterojunction structures as well as a combination of different superlattices. In these studies, we focus on new electrical and optical properties of quantum effects that are not envisioned from the bulk semiconductor properties. In particular, intersubband absorption in both p and n-type $Si_{1-x}Ge_x/Si$ quantum well structures, δ-doped layers in Si are studied. Studies on light emission from strained monolayer layer superlattices as well as devices based on hot carrier effects for structures made of $Si_{1-x}Ge_x/Si$ are performed.

2 Summary of the Most Important Results

With the current ARO support, we have made significant advances in the understanding of optical properties of intersubband transition of $Si_{1-x}Ge_x/Si$ multiple quantum wells, and the fabrication of multiple quantum well infrared detectors operating in the 8-12 μm range. Large many-body effects have been observed in δ-doped Si and heavily doped SiGe/Si quantum well structures. Normal incidence intersubband transitions have been demonstrated for both n and p type SiGe/Si quantum well structures. For potential realization of Si-based light sources we have studied the luminescence from monolayer superlattices and strained alloy layers. In the area of quantum transport, a resonant tunneling transistor has been demonstrated. In the following we highlight the accomplishments made. Details may be referenced to the publications resulting from the past three years efforts listed in section 2.8.

2.1 δ-doped Quantum Wells and Many-Body Effects

In the following, we will describe the important properties of δ- doped quantum wells [1] that we have discovered. The key point is to show that the many-body effects due to δ-doping can be used to tune the transition energy, independent of

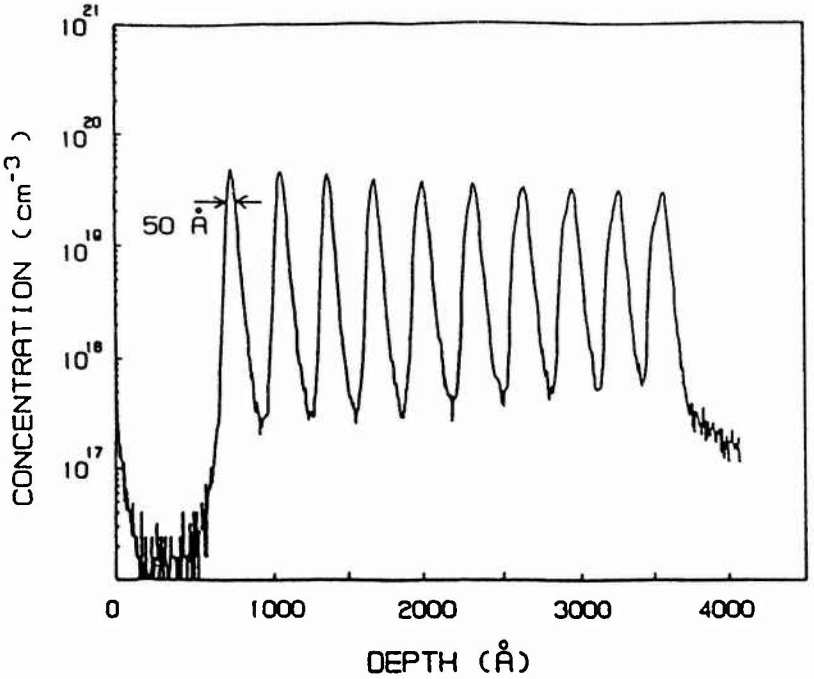

Figure 1: SIMS depth profile of sample A. It reveals 10 periods of boron δ-doped Si layers with a FWHM of about 50 Å.

effective mass. The δ-doping in semiconductors can be viewed as an alternative way of achieving quantum well structures without heterojunctions. The potential profile associated with δ-doping closely resembles that of a parabolic quantum well, due to the finite width of the doped layer. The well thickness and the barrier height can be controlled by the thickness of the doped layer and the doping density. The potential profile and the energy level spectrum in the well is usually obtained by solving the Schrödinger and Poisson's equations self-consistently (Hartree approximation) [2]. For intersubband detector application in the 10 μm range, the population of carriers in such structures needs to be considerably larger (in order to get the required energy level separation) than typically used in heterojunction quantum wells. As a result, the many-body effects play an important role in determining the optical properties of δ-doped quantum wells. A typical structure used in this study consists of an undoped Si buffer layer, followed by 10 periods of 35 $\AA$ of heavily boron-doped Si layers and 300 $\AA$ of undoped Si spacers. Figure 1 shows the (SIMS) depth profile for a typical δ-doped structure (sample A). A full width at half maximum (FWHM) of approximately 50 Å is obtained from the depth profile.

Measured absorption spectra of samples with different doping densities as a function of photon energy are shown in Fig. 2. It can be clearly seen that the absorption

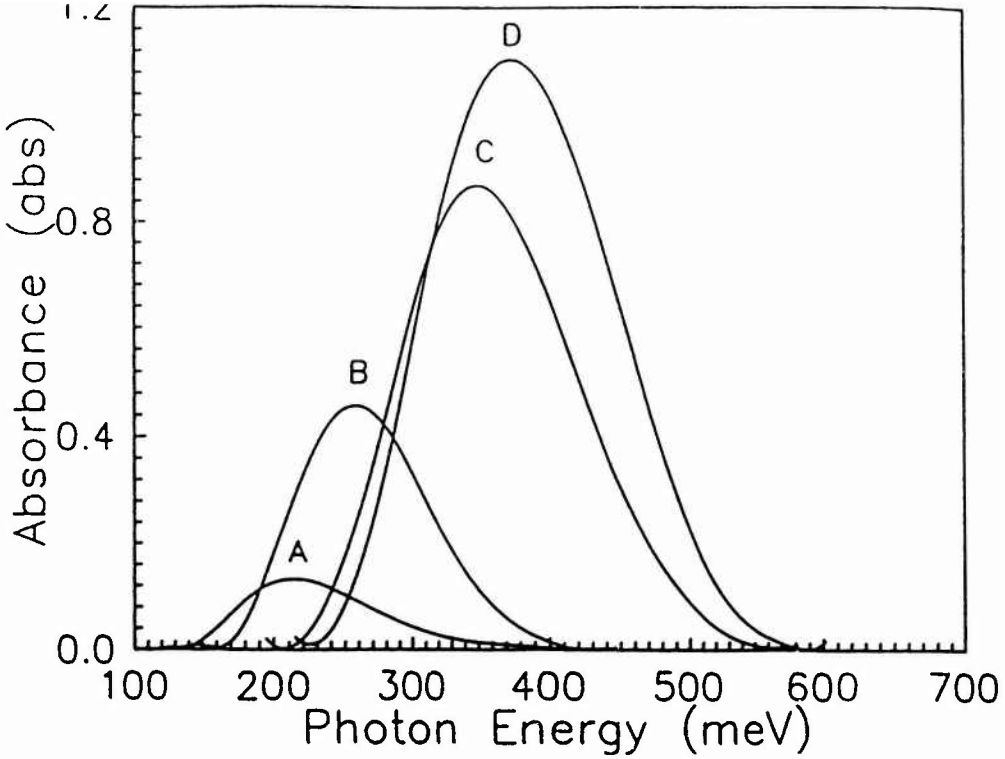

Figure 2: Absorption spectra of the four samples as a function of photon energy at 300 K. The set of curves is due to different doping concentrations.

spectra shift towards the high energy regime with increasing absorption as the doping density is increased. The shift of the absorption peak is mainly due to the increase of the potential well depth at high doping densities. The widths of the absorption peaks are more than an order of magnitude larger than those observed in GaAs/AiGaAs quantum well structures, typically about 10 meV. The polarization dependence of the spectra shows a similar behavior as in the case of multiple quantum wells discussed above, indicating the one dimensional nature of the potential.

The experimental peak positions along with the calculated values using a multi-band self-consistent calculation (Hartree approximation) are shown in Fig. 3. These values are considerably smaller than the experimental values shown by the open circles. The solid curve in the Fig. 3 shows the incorporation of the many-body effects (i.e., Hartree-Fock approximation) to the calculated energy level separation. This brought the calculated and experimental peak positions to a reasonably close agreement. The significance of this work demonstrates the substantially large many-body effects of SiGe than those of the GaAs-based system.

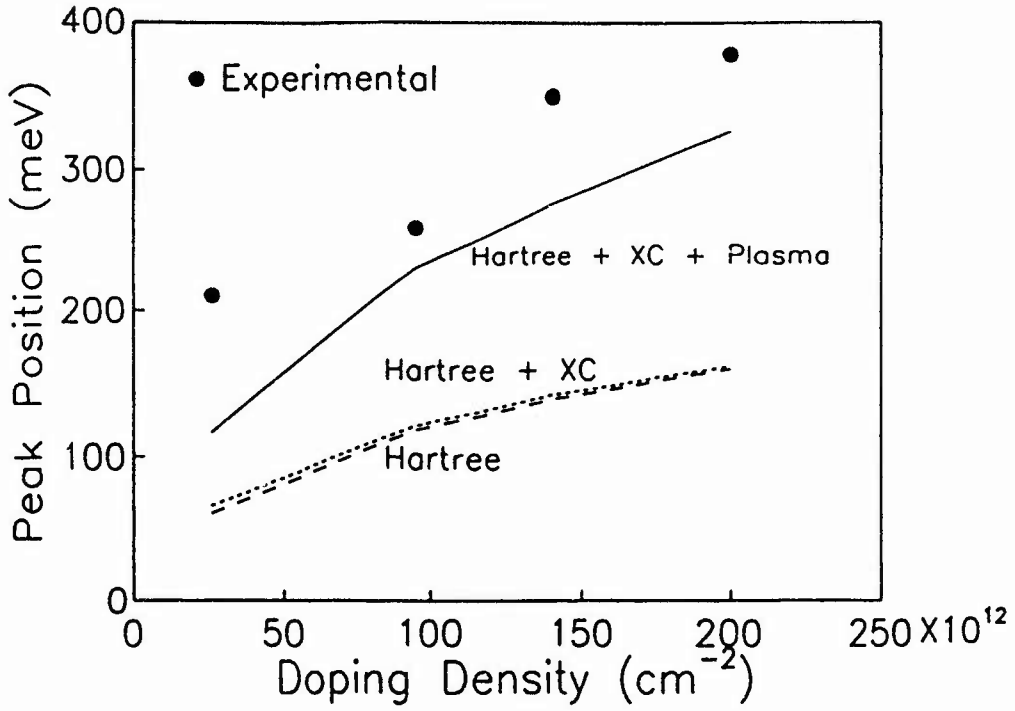

Figure 3: Subband separation as a function of doping density (a) experimental data (dashed curve with open circles), calculated results using (b) using the Hartree approximation (dashed curve), and (c) the Hartree-Fock approximation (solid curve).

2.2 Intersubband Absorption in SiGe/Si Quantum Wells

The following examples will demonstrate the work to date in the intersubband transition and ability to quantify the polarization dependence [3]. The work described below is for p-type (100) and the transition obtained is between two heavy hole subbands and thus has the same selection rule as the AlGaAs/GaAs conduction subband transition. In the case of SiGe grown on Si, most of the band offset appears in the valence band and the intersubband absorption of holes can be more conveniently studied. The transmission spectrum of the sample is taken at room temperature using a Fourier transform infrared (FTIR) spectrometer. In the measurement, a waveguide structure of 5 mm long and 0.5 mm thick is employed (see inset of Fig. 4) in order to enhance the absorption.

Measured absorption spectra as a function of energy using the waveguide structure are shown in Fig. 4. The set of curves are due to different polarization angles of the infrared beam and the zero degree corresponds to the polarization of the beam along the growth direction. The strength of the intersubband absorption decreases as the polarization of the infrared beam is rotated from the perpendicular direction

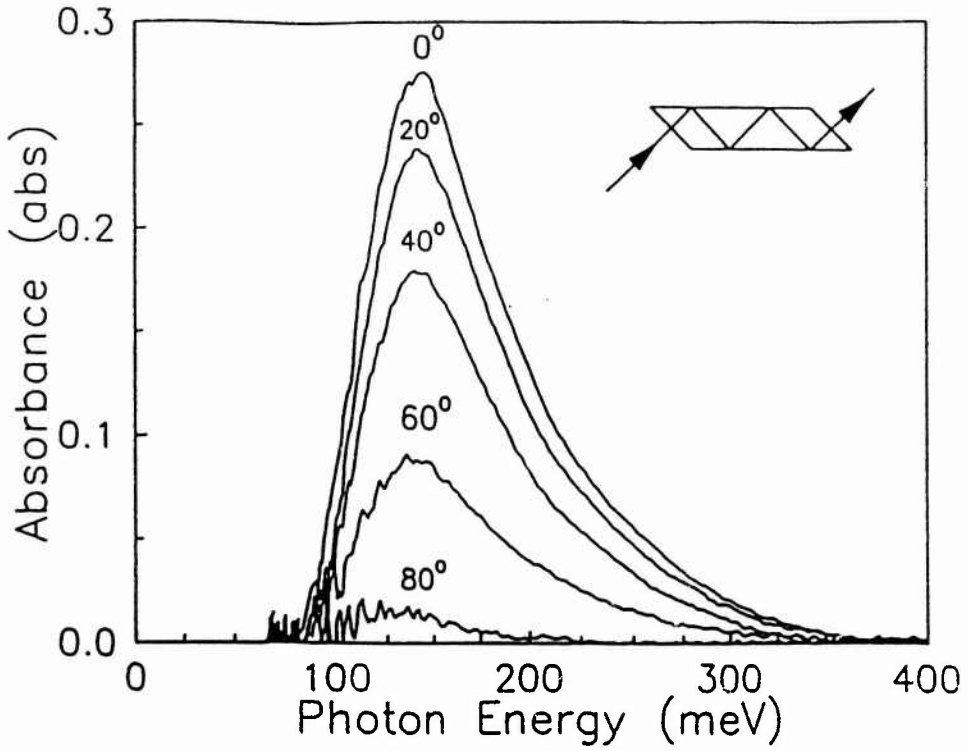

Figure 4: Measured absorption spectra as a function of energy for different polarization angles of the incident infrared beam. The absorption strength at large polarization angles is shown to decrease in accordance with the selection rules of intersubband transition at the Γ- point. The inset shows the waveguide structure used in the measurement.

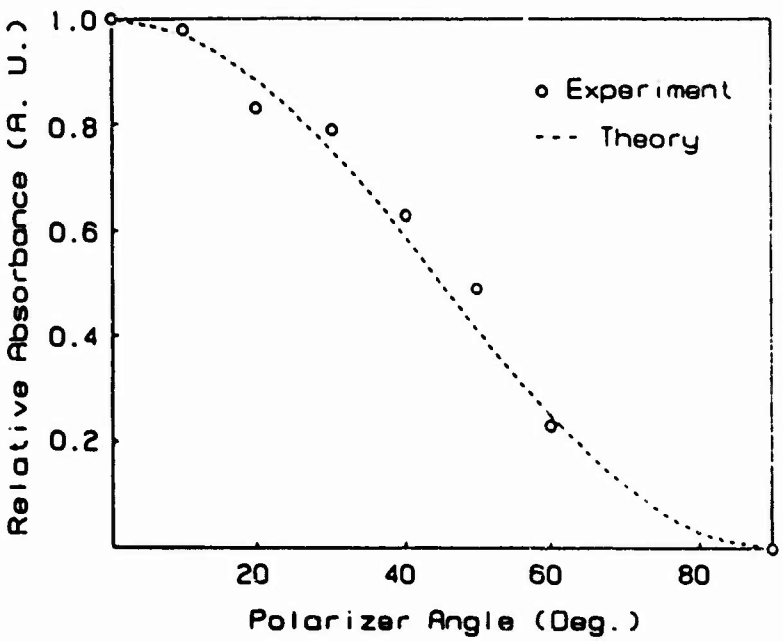

Figure 5: Normalized absorption strength as a function of the polarization of the incident infrared beam. The zero degree corresponds to the polarization along the growth direction of the structure. The dashed curve shows the theoretically expected $\cos^2\phi$ dependence.

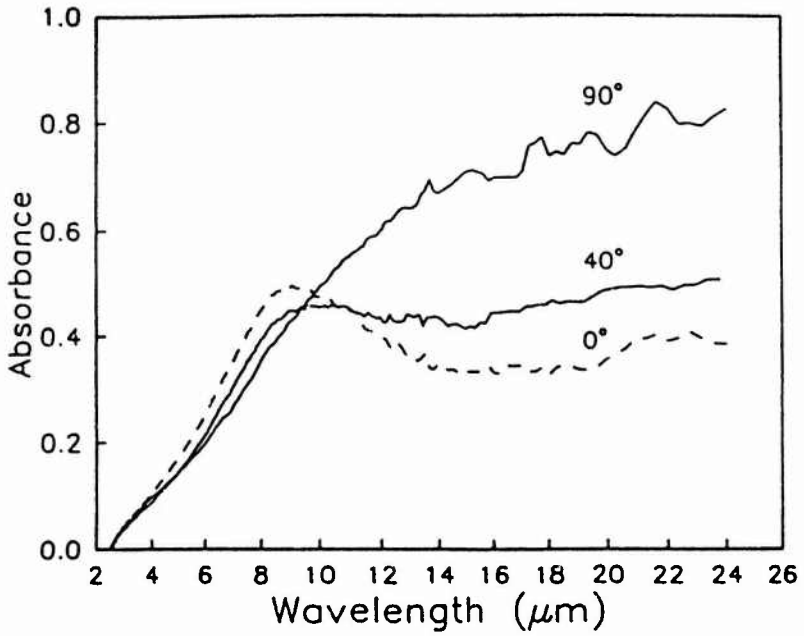

Figure 6: Measured FTIR spectrum at 300 K. Absorption spectra at three different polarization angles are shown. At the 0° polarization, a broad peak near 9 μm is seen. This peak is due to a heavy hole intersubband transition. The 90° case shows a stronger background absorption most likely due to free carrier absorption, but the peak seen at the 0° polarization is not visible.

towards the parallel direction of the plane of layers. Figure 5 illustrates the relative absorption strength as a function of the polarizer angle ϕ and the data follow the $\cos^2\phi$ dependence (dashed curve), in good agreement with the selection rule of the intersubband transition. The estimated oscillator strength using the absorption data is about 0.98, which is in good agreement with the calculations. The value is also close to that obtained for intersubband absorption in III-V based quantum well structures which are in the 0.5 to 1.2 range.

2.3 Detector Application

We have investigated the potential application of SiGe/Si multiple quantum wells for infrared detectors [4, 5]. The use of Si-based quantum well structures has an added advantage due to the potential for integrating with Si signal processing electronics in a monolithic manner. The Ge composition and the well thickness are selected to have the heavy hole bound state inside the well and the first extended excited state close to the continuum of the barriers for detector application.

Figure 6 shows the room temperature absorption spectrum for different polarization angles as a function of wavelength using a 45° multipass waveguide structure with dimensions of 4 mm long and 0.5 mm wide. At the 0° polarization, the incoming photon electric field has components both along the growth direction (z-direction) and parallel with the growth plane (xy-plane). In this case, the absorption spectrum consists of a relatively broad peak at near 9 μm superimposed on a monotonically increasing background as the wavelength is increased. On the other hand at the 90° polarization where the field is polarized only along xy-plane, the absorption shows the similar trend as the 0° case, but the absorption strength is stronger and the peak at 9 μm is no longer visible. As the polarization angle increases, the peak absorption decreases (characteristics of intersubband transition at the Γ-point) while the background absorption increases. The absorption spectrum at the 90° polarization in Fig. 6 is mostly due to two dimensional free carrier absorption. In this case, the photon absorption occurs via phonon or impurity scattering to conserve the momentum. As the polarization angle increases, the photon field in xy-plane increases while the field in the z-direction decreases. This causes an increase of free carrier absorption and a decrease of intersubband absorption as the polarization angle increases.

Mesa diodes of 200 μm in diameter with a 45° facet on the edge of the wafer as shown in the inset of Fig. 7 are fabricated for the study of photoresponse. The infrared is illuminated on the facet at the normal such that the incident angle on the multiple quantum well structure is 45°. The photo-signals are measured at two different polarization angles of 0° and 90°. Figure 7 shows the photocurrents at the 0° and 90° polarizations at 40 K, with a 2 V bias across the detector. In the 0° polarization case, a peak is found at near 8.6 μm which is in agreement with the FTIR absorption spectra, except the peak position moves slightly to a lower wavelength because of the use of different temperatures in the two measurements. The full width at half maximum (FWHM) is about 80 meV and is also in agreement with the absorption spectra, while for the 90° polarization, the peak at near 7.2 μm is observed with a similar FWHM. For the latter, the shift of the peak to a shorter wavelength may be due to the sharing of phonon energy with momentum conserving processes such as phonon or impurity scattering. The peak photocurrent found at

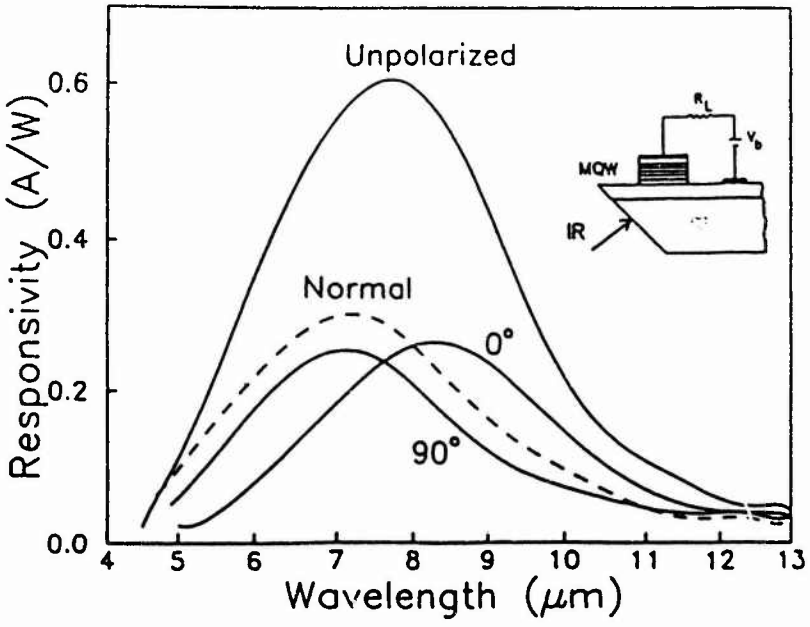

Figure 7: Photoresponse at 40 K for two polarizations angles with a 2 V bias applied across the detector. Infrared is illuminated on the facet at the normal such that the incident angle on the multiple quantum well structure is 45° as shown in the inset.

the 0° polarization case disappears in this case. The photoresponse for both cases are about the same, 0.3 A/W. Fig. 7 shows the photocurrent along with the result obtained from a unpolarized beam. In the latter case, a peak is found at near 7.5 μm and the photocurrent is about 0.6 A/W, approximately the sum of two polarization cases.

It is clear that for the 0° polarization case, the photocurrent is due to intersubband transition between two heavy hole subbands and also partially due to internal photoemission of holes excited via free carrier absorption. For the 90° polarization case, intersubband transition is forbidden but free carrier absorption is stronger than that of the 0° polarization case because entire photon electric field lies in the xy-plane. The photocurrent in this case is believed to be due to internal photoemission of free carriers.

For the present not yet optimized detector, a quantum efficiency of $\eta \sim 14$ % is obtained for the polarized light. For the unpolarized case, the photocurrent is the sum of both intersubband transition and the photoemission due to free carriers.

2.4 Normal Incidence Intersubband Absorption

One of the major drawbacks of intersubband transition for the Γ valley is that the normal incidence light cannot be detected. In order to circumvent this limitation, we have explored several alternative normal incidence concepts in both n-type and p-type SiGe/Si MQWs. For n-type, this results from the coupling of light with the off-diagonal components of the electron effective mass tensor, or the tilted energy ellipsoids being away from the Γ-point [6]. The intersubband absorption at the Γ-point requires a component of photon electric field along the quantum well direction. For the (100) oriented Si substrate the condition applies since the (100) directions lie in the principal directions of the constant energy ellipsoids. On the other hand, for a similar structure grown on a (110) or other than (100) Si substrate, the non-zero off-diagonal effective mass components provide the coupling of normal incident light to induce the intersubband transition. Figure 8 shows the intersubband absorption in δ-doped quantum wells for (100) and (110) oriented substrates. The polarization dependence absorption data for the structure grown on (110) Si substrate confirms the normal incidence transition. Next, we will discuss similar transitions in the valence band due to band mixing.

For p-type, with a significant band coupling from the conduction Γ-point, it is possible to have transitions between different hole bands (for example, between the heavy and light hole bands) [7]. This is particularly important in the case of SiGe grown on Si substrate where the strain reduces the bandgap, resulting in a strong coupling between the conduction and valence bands as the Ge composition is increased. The evaluation of the optical matrix element using **k·p** approximation indicates the strength of this transition is inversely proportional to the square of the bandgap, which reduces as the Ge composition is increased.

In the experiment, two $Si_{1-x}Ge_x$/Si multiple quantum well structures with 30% and 60% Ge compositions were employed. Figure 9 shows the room temperature absorption spectra at the 90° polarization (i.e., normal incidence) for the two samples as a function of wavelength using a 45° multipass waveguide structure, 5 mm long and 0.5 mm wide. For clarity, we have subtracted the monotonically increasing background absorption mainly due to free carrier absorption in the doped quantum

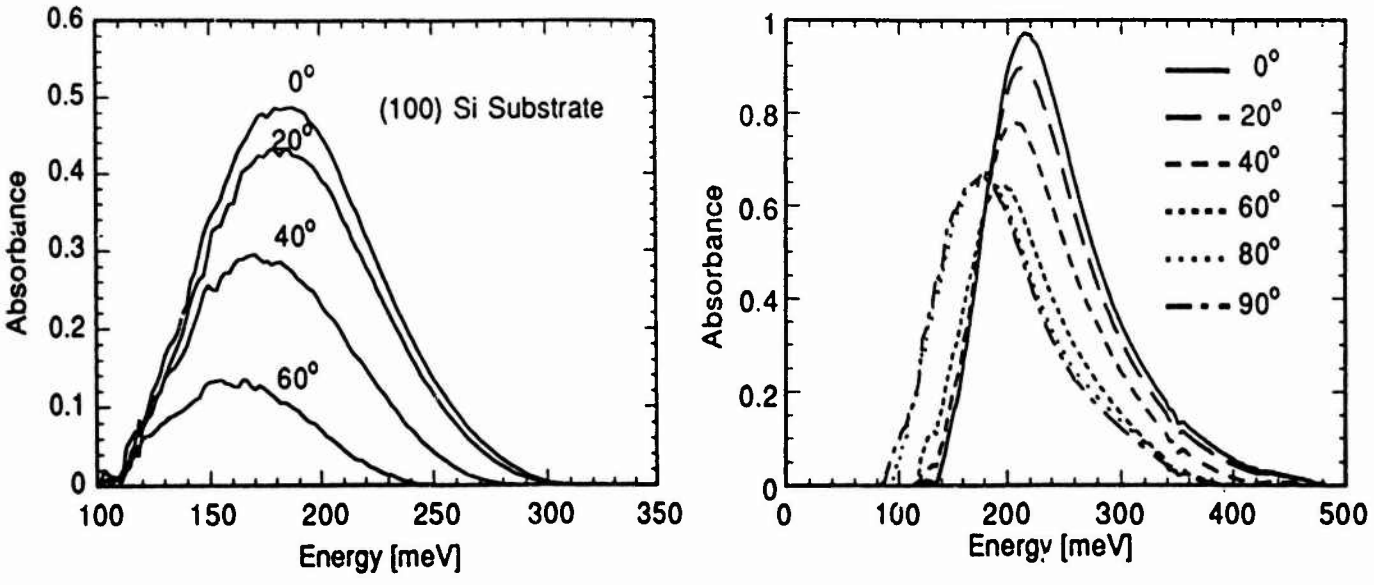

Figure 8: Intersubband absorption by δ-doped structures grown on (100) and (110) oriented Si substrates. The polarization dependence data of (110) structure shows the normal incidence absorption.

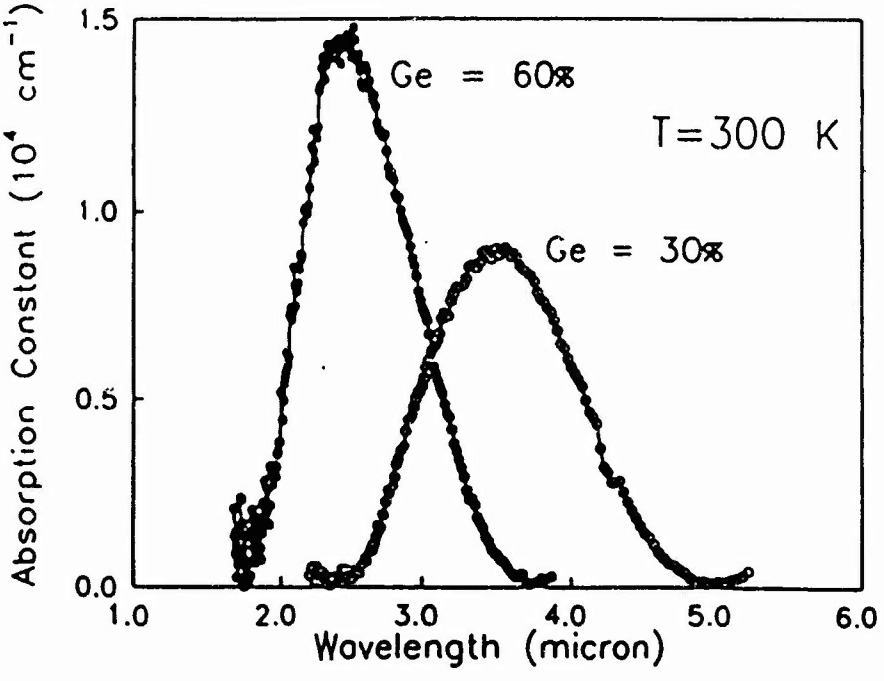

Figure 9: Intervalence band transition as a function of wavelength for two samples with different Ge compositions. The shift of the peak position is due to the splitting of the hole bands due to strain.

wells. The magnitude of the observed absorption coefficient ($\sim 10^4$ cm^{-1}) is as large as typically observed in direct gap semiconductors. As shown in Fig. 9, peaks in the absorption were observed at 3.4 and 2.5 μm for samples 30% and 60%, respectively. This normal incidence absorption is mainly due to excitation of holes from the heavy hole ground state to the ground state of the split-off band and the continuum hole subbands. The enhancement of the absorption with increasing Ge composition is due to the reduction of the bandgap at the Γ-point as mentioned before.

Our research shows that normal incidence intersubband transition can be obtained for both n and p-type SiGe/Si quantum wells. The work leads to an advance in the understanding of intersubband transition.

2.5 Optical Properties of Monolayer Si_mGe_n Superlattices

The optical properties of monolayer Si_mGe_n superlattices have been investigated by photoluminescence (PL) spectroscopy [8, 9]. The aim of this work is to understand the band-folding effects due to the short superlattice periodicity. In order to distinguish bandgap-related luminescence from defects and dislocations, the samples were passivated with atomic hydrogen. Fig. 10 shows the PL spectra, for example, of a 16×4 SL before and after passivation. The broad background luminescence in the low energy region is a characteristic of the D lines ascribed to dislocations in a plastically deformed SiGe buffer layer. Using a step by step chemical etching, the broad peak was shown to originate from the buffer layer. Upon passivation, this broad signal was considerably reduced in intensity and only two well defined peaks remained from the original spectrum. The 61 meV difference in energy between the two peaks was close to the Si-Si optical phonon vibration energy as measured by a Raman experiment. Thus the H-passivation study appears to confirm that the observed peaks at 1.026 eV and 0.965 eV are due to transitions in the SL. Similar behavior was also observed for the 14×4 superlattice with transitions at 0.998 eV and 0.940 eV. The lowering of the transition energy is due to the larger average Ge composition in the 14×4 superlattice compared with the 16×4 superlattice.

To further support the assertion that the 1.026 eV and 0.965 eV lines for the 16×4 SL (0.998 eV and 0.940 eV for the 12×4 SL) are superlattice-related, we have

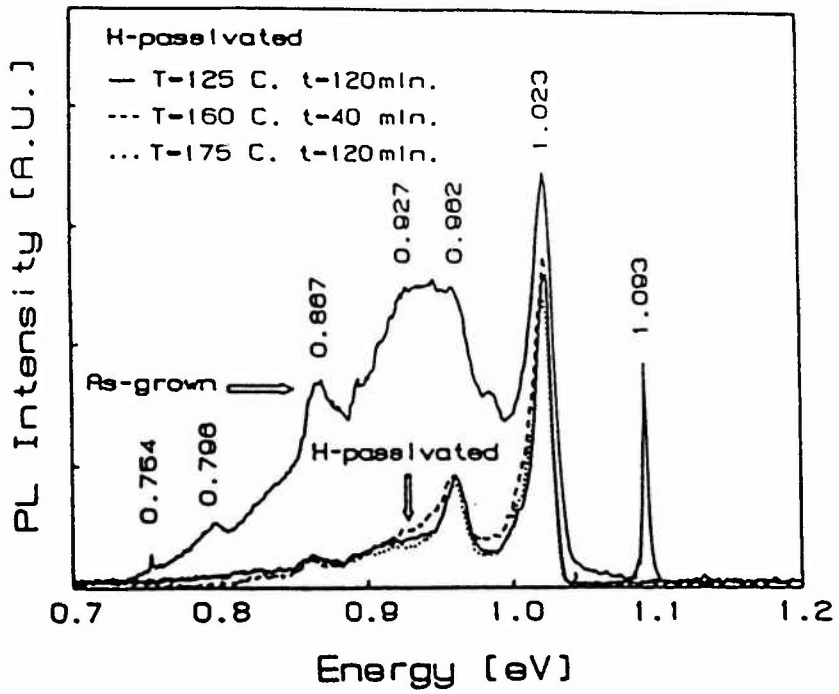

Figure 10: As-grown and hydrogenated photoluminescence spectra of a 16×4 superlattice. Hydrogenated spectra for three different temperatures and times are presented.

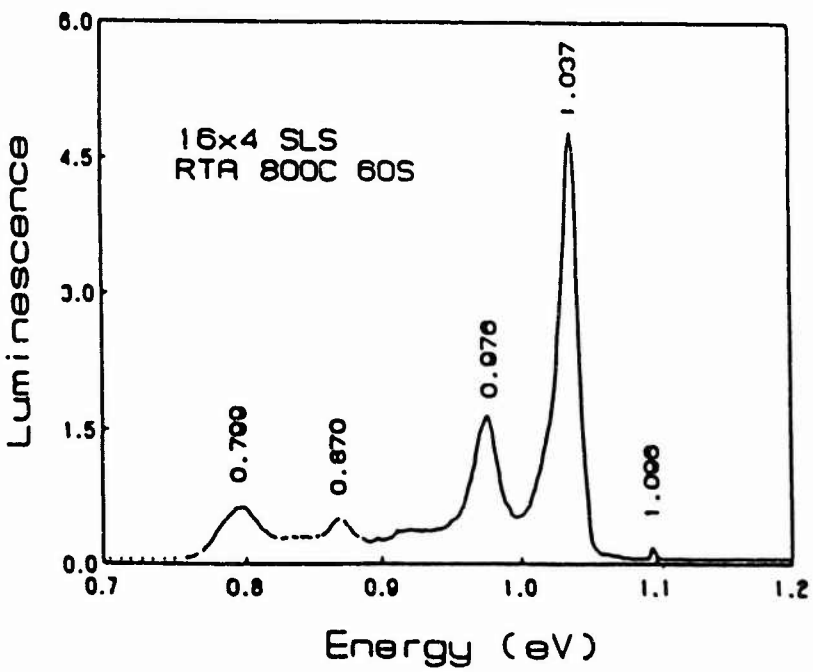

Figure 11: PL spectrum of the 16×4 SLS after an 800 °C, 60 second RTA. The peaks at 0.976 and 1.037 eV correspond, respectively, to the 0.965 eV shoulder and the 1.026 eV peak of the spectrum of the as-grown sample. The features at 0.799 and 0.870 eV are due to the buffer layer.

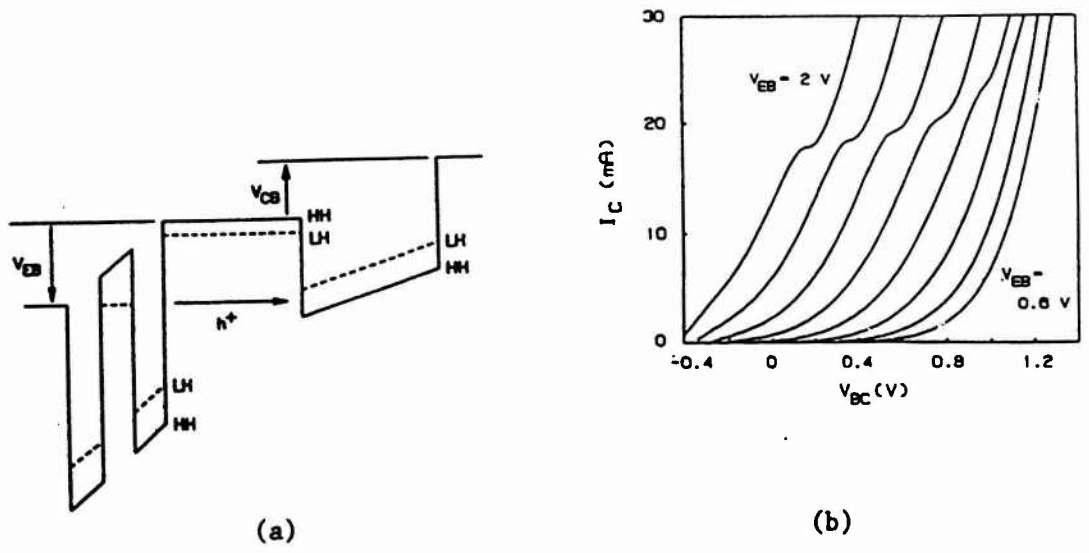

Figure 12: (a) Valence band diagram of the transistor under an external bias showing the conductance process, and (b) collector current I_C of the device as a function of V_{BC} at 77 K in a common base configuration. V_{EB} is the parameter with a step of 200 mV.

performed rapid thermal annealing (RTA) on the samples. The spectrum of the 16×4 SL after a RTA anneal at 800°C for 60 seconds is shown on Fig. 11 and is very similar to the spectrum obtained after hydrogenation. The two main peaks have shifted to higher energy due to the interdiffusion of the Si and Ge atoms at the interfaces. It is worth noting that the energy separation between the two peaks remains at 61 meV.

From these results, it is believed that the effect of the artificially introduced periodicity on the band structure is responsible for the observed superlattice PL signals, although no direct gap nature is confirmed. However, the observation of superlattice transition is a step towards better understanding of the light emission of zone-folded structures.

2.6 Resonant Tunneling Transistor

There is a growing interest in the application of resonant tunneling transistors due to expected high frequency response into the THz range. We have investigated such a transistor using holes in Si/Ge system since most of the band offset appears at the valence band [10]. Figure 12(a) shows schematically the band diagram under an

external bias. When the emitter is biased positively with respect to the base, holes are injected into the base through the double barrier resonant tunneling emitter with an excess hole energy relative to the valence band maximum of the base. The holes injected into the base are then transferred near-ballistically to the collector. The collector barrier prevents injection of the holes initiated from the valence-band of the base to the collector when V_{BC} is applied, while allowing the injected hot holes from the emitter to go through to the collector if these hot holes have higher energies than the collector (light hole) barrier height.

In Fig. 12(b), a set of collector currents (I_C) is shown as a function of the base-collector voltage (V_{BC}) at 77 K, with V_{EB} as a parameter. The rightmost curve corresponds to V_{EB} = 600 mV and others are for an incremental step of 200 mV. At V_{EB} = 600 mV, no NDR is observed since a large portion of the collector current comes from the base. As the emitter bias is increased, the injection current from the emitter becomes the dominant source of the collector current, the NDR becomes apparent, and the NDR ratio increases with V_{EB}.

2.7 Summary

In summary, in the performance period we have studied the intersubband transitions in δ-doped quantum well structure in Si. The importance of many-body effects on the transition energy have been demonstrated for the first time. In the case of SiGe/Si heterostructures, intersubband transition between quantized states has been demonstrated for the first time. Infrared detectors operating near 10 μm have also been fabricated. In addition to intersubband transition in the valence band, a new transition between different hole bands is discovered. The advantage of this transition is to have normal incidence infrared detection. Similarly, for n-type quantum well structures grown on Si (110) substrates, normal incidence transitions have been observed due to non-vanshing components of the effective mass tensor. As step towards achieving Si-based light sources, we have studied the luminescence of strained SiGe layers. The luminescence originated from the alloy was discriminated from those of dislocations using hydrogen passivation and progressively etching of the structure. In the

study of transport properties we have demonstrated a resonant tunneling transistor with controllable negative resistance.

2.8 List of Publications

Manuscripts published or submitted

Rhee, S. S., Chang, G. K., Carns, T. K., and Wang, K. L., "SiGe Resonant Tunneling Hot Carrier Transistor", Proceedings IEEE/IEDM, 27.4.1, 651-654, (1989).

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4 Report of Inventions

"Normal Incidence Long Wavelength Infrared Detectors Using Intervalence-subband Transition in $Si_{1-x}Ge_x$/Si Multiple Quantum Wells".

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