Extended Abstracts of the 1993 International Conference on Solid State Devices and Materials, Makuhari, 1993, pp. 500-502

Photoluminescence of $Si_xGe_{1-x}/Si_yGe_{1-y}$ Multiple Quantum Wells Grown on Ge(100) Substrates

Koichi Terashima, Douglas Tweet, Keiko Miyanaga, Toru Tatsumi, and Michio Tajima*
Microelectronics Res. Labs., NEC Corporation,
34 Miyukigaoka, Tsukuba 305, JAPAN
*Institute of Space and Astronautical Science,
3-1-1, Yoshinodai, Sagamihara 229, JAPAN

We have fabricated strained SiGe layers on Ge(100) substrates and measured the photoluminescence (PL) spectra. Band-edge emission from the SiGe alloy has been observed for $Si_xGe_{1-x}/Si_yGe_{1-y}$ multiple quantum wells (MQW) due to recombination of bound excitons in the SiGe alloy having the smaller band gap energy (i.e. the smaller of x and y). From the positions of the observed PL lines, we can evaluate the band gap energy of the strained SiGe alloy layers. The resulting band gap energies are smaller than those of bulk SiGe alloys and agree well with the theoretical values for strained layers. We have also observed emission due to dislocations at the interface.

1. Introduction

Strained SiGe epitaxial layers have attracted much attention in recent years because of the high potential for device applications. Fundamental parameters such as the band gap energy are very important when the materials are used for device fabrication. However, knowledge of these parameters, especially the effect of the strain, is still insufficient. In the case of a Ge substrate, the strain in the SiGe layer is tensile while it is compressive for a Si substrate. Consequently, the physical properties of the SiGe layers are expected to be different for these two substrates. According to the calculation by People[1], the band gap energy of SiGe on Ge(100) is smaller than the case of the unstrained bulk. Also, when the Si content of the alloy is smaller than about 15%, the band gap energy increases with the Si content, after which it decreases.

Photoluminescence (PL) is a powerful method for investigating the physical properties of solids. We have reported PL of SiGe alloy layers on Si(100) and discussed the effect of strain on the band gap energy of SiGe[2]. Recently, many authors have reported on PL of SiGe epitaxial layers[3-8]. However, most work has been done on Si substrates. Therefore, in this study, we have fabricated strained SiGe layers on Ge(100) substrates and measured the PL spectra in order to clarify the effect of strain on the band gap energy.

2. Experiments

The samples were grown on 50-mm-diam Ge(100) wafers with a resistivity of 50 Ωcm by ultra high vacuum chemical vapor deposition (UHV-CVD) using Si_2H_6 and GeH_4 at a substrate temperature of 480 °C. We have fabricated two types of samples. One is a single SiGe alloy layer without any cap and the other is a 10 period $Si_xGe_{1-x}/Si_yGe_{1-y}$ multiple quantum well (MQW). The structures and the alloy compositions were investigated by transmission electron microscopy (TEM) and x-ray diffraction (XRD). The XRD measurement confirmed that the SiGe layers are strained. Typical structures are listed in Table I.

In the PL measurement, the samples were immersed in liquid He and excited by the 488 nm line of an Ar ion laser. The emission from the samples was analyzed by a 32 cm grating monochromator with a 600 groove/mm grating blazed at 1 μm and detected by a cooled Ge or a cooled PbS detector.

Table I. Structures and alloy compositions of the samples.

Sample	Type	Thickness of Si_xGe_{1-x}	x	Thickness of Si_yGe_{1-y}	y	Period
A	Single layer	4600 Å	0.07			1
B	MQW	80 Å	0.08	85 Å	0.15	10
C	MQW	62 Å	0.20	67 Å	0.06	10

3. Results and discussion

Representative PL spectra of SiGe on Ge(100) are shown in Fig. 1 together with the PL of a Ge substrate. In the spectrum of the Ge substrate, the emission lines labelled BE and EHD are due to the recombinations of bound excitons and electron-hole drops (EHD), respectively. The superscript NP indicates the no-phonon (NP) transition and TA and LA indicate the transitions assisted by transverse acoustic (TA) phonons and longitudinal acoustic (LA) phonons, respectively.

For the single SiGe layer on a Ge substrate (sample A), the PL spectrum is almost the same as that of the Ge substrate except the relative intensity of the BE line and the EHD line. In this case, we cannot observe the band-edge emission of SiGe. As the band gap energy of Ge is smaller than that of strained SiGe for this Si content, most of the excited carriers move to the Ge substrate before they recombine. Thus, we observe only emission from the Ge substrate.

On the other hand, in the PL spectra of MQWs (samples B and C), new lines labelled X appear in the energy region above the band-edge emission from the Ge substrate. The energy separation between the X^{NP} line and the $X^{TO(Ge-Ge)}$ line is 34 meV. This value is almost the same as the energy of the Ge-Ge mode of the transverse optical (TO) phonon in unstrained SiGe alloy[9], hence the indicated assignments.

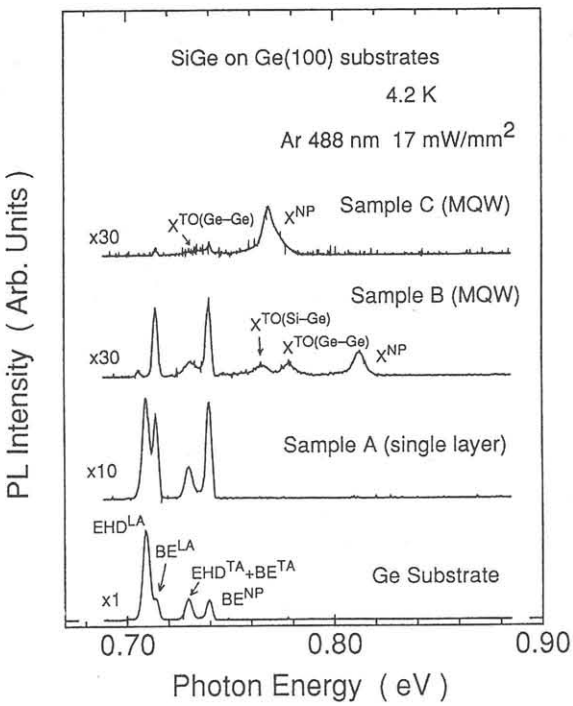

Fig.1. Photoluminescence spectra of SiGe layers on Ge(100) substrates. Spectral bandpass is 6 nm. The notation "×10" indicates the original intensity is magnified by a factor of 10.

Similarly, the separation between the X^{NP} line and the $X^{TO(Si-Ge)}$ line (47 meV) is almost the same as the energy of the Si-Ge mode of the TO phonon. Considering the energy separation between the X lines as well as the line shape, the impurity concentrations in the SiGe layers (mainly boron, ~10^{16} cm^{-3}) and the low temperature of 4.2 K, we assign these X lines to the recombinations of bound excitons for boron in the SiGe layers. The three X lines are the NP line of the bound exciton and its phonon replicas. Therefore we have observed band-edge emission of SiGe due to the carrier confinement in the quantum wells. The emission is from the SiGe alloy having the smaller band gap energy (i.e. the smaller of x and y, see Table I).

From the positions of the observed PL lines, we can evaluate the band gap energy of the strained SiGe alloy layers. The band gap energy E_g is given by

$$E_g = E_{XNP} + E_{BE} + E_{FE} - E_{conf}, \qquad (1)$$

where E_{XNP} is the energy position of the X^{NP} line, E_{BE} the binding energy of the bound exciton, E_{FE} the binding energy of the free exciton, and E_{conf} the energy shift of the band gap due to the quantum confinement effect. Unfortunately, the exact values of these parameters are unknown except E_{XNP}, which is obtained directly from the PL measurement. The binding energy of the bound exciton, E_{BE}, can be obtained directly from the PL measurement if the free exciton line is observable. However, in the present work, we cannot distinguish the free exciton line even for high excitation power density or at higher temperature. The reported value of E_{BE} for boron is 4.6 meV and 1 meV in the case of Si and Ge, respectively[10]. The binding energy of the free exciton is 14.7 meV for Si and 4.15 meV for Ge[10]. We evaluated E_{BE} and E_{FE} for the SiGe alloy assuming that these values are proportional to the alloy composition.

The energy shift of the band gap due to the carrier confinement effect, E_{conf}, must also be taken into account. This effect has been reported for SiGe/Si quantum wells[4-8]. The energy shift is affected mainly by the well width and the band offset. According to People's calculation[1], the band offset of SiGe/Ge is 10-40 meV for the conduction band and 20-100 meV for the valence band in the alloy composition range of this work. These values are small compared with SiGe/Si. We have estimated that E_{conf} is of the order of several meV in this work. The band gap energies of SiGe obtained from the PL measurement using equation (1) are listed in Table II. The theoretical calculation by People[1] is given for a temperature of 77 K while our PL measurement has been done at 4.2 K. The red shift of the band gap of SiGe due to the

Table II. Band gap energy E_g of Si_xGe_{1-x} alloys on Ge(100).

Alloy composition x	Position of X^{NP} line	E_g obtained from PL (4.2 K)	E_g calculated for strained layer (77 K)[a)]	E_g obtained for bulk (4.2 K)[b)]
0.08	0.811 eV	0.81 eV	0.80 eV	0.85 eV
0.06	0.768 eV	0.77 eV	0.77 eV	0.82 eV

a) Reference 1.

b) Reference 9.

increase of the temperature from 4.2 K to 77 K is about 3-5 meV considering data reported for Si and Ge[10]. The band gap energies obtained in this work are smaller than those of bulk SiGe alloys and agree well with the theoretical values for strained layers calculated by People.

For sample C in Fig. 1, the intensity of the X^{NP} line relative to the band-edge emission of the Ge substrate is strong and the $X^{TO(Si-Ge)}$ line cannot be observed. PL spectra of sample C are shown in Fig. 2 for different excitation power densities. New emission bands appear as the excitation power density increases. In TEM observations we have found dislocations at the interface between the substrate and the first epitaxial layer ($Si_{0.20}Ge_{0.80}$, see Table I). The energy positions of the new emission bands agree well with those of dislocation-related D-lines in bulk $Si_{0.20}Ge_{0.80}$. Therefore we consider these new emission bands to be due to the dislocations at the interface.

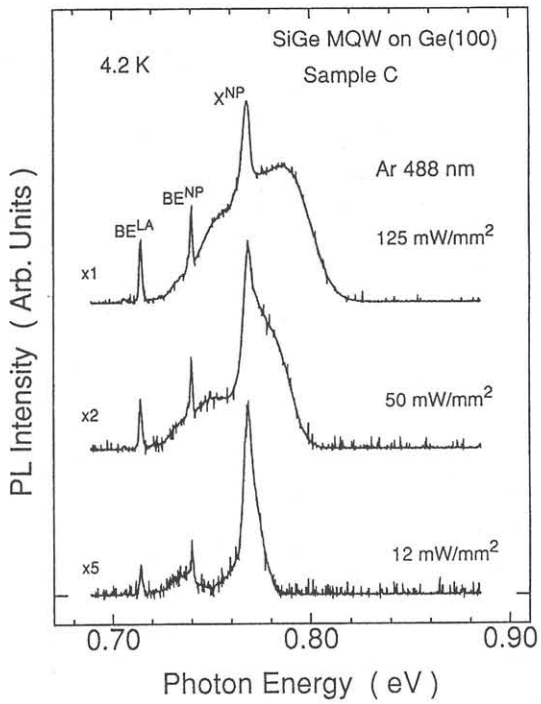

Fig. 2. Photoluminescence spectra of SiGe MQW on Ge(100) (sample C) for different excitation power densities. Spectral bandpass is 6 nm.

4. Conclusions

We have observed band-edge emission of SiGe from $Si_xGe_{1-x}/Si_yGe_{1-y}$ MQW, due to recombination of bound excitons in the quantum well. From the positions of the observed PL lines, we have evaluated the band gap energy of the strained SiGe alloy layers. The resulting band gap energies are smaller than those of bulk SiGe alloys and agree well with the theoretical values for strained layers. We have also observed emission due to dislocations at the interface.

Acknowledgement

We are grateful to Y. Matsumoto and H. Ono for their helpful discussions and great encouragement. We would like to thank M. Warashina for his help in the PL measurement.

References

1) R. People, Phys. Rev. B **34** (1986) 2508.
2) K. Terashima, T. Tatsumi, and M. Tajima, Appl. Phys. Lett. **57** (1990) 1925.
3) J.-P. Noel, N. L. Rowell, D. C. Houghton, and D. D. Perovic, Appl. Phys. Lett. **57** (1990) 1037.
4) J. C. Sturm, H. Manoharan, L. C. Lenchyshyn, M. L. W. Thewalt, N. L. Rowell, J. -P. Noel, and D. C. Houghton, Phys. Rev. Lett. **66** (1991) 1362.
5) D. J. Robbins, L. T. Canham, S. J. Barnett, A. D. Pitt, and P. Calcott, J. Appl. Phys. **71** (1992) 1407.
6) X. Xiao, C. W. Liu, J. C. Sturm, L. C. Lenchyshyn, M. L. W. Thewalt, R. B. Gregory, and P. Fejes, Appl. Phys. Lett. **60** (1992) 2135.
7) L. Vescan, A. Hartmann, K. Schmidt, Ch. Dieker, H. Luth, and W. Jager, Appl. Phys. Lett. **60** (1992) 2183.
8) S. Fukatsu, H. Yoshida, A. Fujiwara, Y. Takahashi, Y. Shiraki, and R. Ito, Appl. Phys. Lett. **61** (1992) 804.
9) J. Weber and M. I. Alonso, Phys Rev. B **40** (1989) 5683.
10) *Data in Science and Technology, Semiconductors Group IV Elements and III-V Compounds* (Springer-Verlag Berlin Heidelberg 1991) and references therein.