Growth and electron effective mass measurements of strained Si and Si_{0.94}Ge_{0.06} on relaxed Si_{0.62}Ge_{0.38} buffers grown by rapid thermal chemical vapor deposition

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Abstract

We report the growth and the electron cyclotron resonance measurements of n-type Si/Si_{0.62}Ge_{0.38} and Si_{0.94}Ge_{0.06}/Si_{0.62}Ge_{0.38} modulation-doped heterostructures grown by rapid thermal chemical vapor deposition. The strained Si and Si_{0.94}Ge_{0.06} channels were grown on relaxed Si_{0.62}Ge_{0.38} buffer layers, which consist of 0.6 μm uniform Si_{0.62}Ge_{0.38} layers and 0.5 μm compositionally graded relaxed SiGe layers from 0 to 38% Ge. The buffer layers were annealed at 800°C for 1 h to obtain complete relaxation. A 75 Å Si(SiGe) channel with a 100 Å spacer and a 300 Å 2 × 10¹⁹ cm⁻³ n-type supply layer was grown on the top of the buffer layers. The cross-sectional transmission electron microscope reveals that the dense dislocation network is confined to the buffer layer, and relatively few dislocations terminate on the surface. The plan-view image indicates the threading dislocation density is about 4 × 10⁶ cm⁻². The far-infrared measurements of electron cyclotron resonance were performed at 4 K with the magnetic field of 4–8 T. The effective masses determined from the slope of the center frequency of the absorption peak versus applied magnetic field plot are 0.203m₀ and 0.193m₀ for the two dimensional electron gases in the Si and Si_{0.94}Ge_{0.06} channels, respectively. The Si effective mass is very close to that of a two dimensional electron gas in an Si MOSFET (0.198m₀). The electron effective mass of Si_{0.94}Ge_{0.06} is reported for the first time and is about 5% lower than that of pure Si.

Keywords: Graded relaxed buffer; SiGe; Cyclotron resonance; Electron effective mass

1. Introduction

Recently, there has been remarkable progress in SiGe technology. The f_T (cutoff frequency) and f_{max} (maximum frequency of oscillation) of Si/SiGe heterojunction bipolar transistors (HBT) have reached 117 GHz [1] and 160 GHz [2], respectively. This possibly offers Si-based ICs with low cost and high speed to wireless communication markets. Moreover, the electron mobility and hole mobility of 5.2×10^5 [3] and 5.5×10^4 cm² V⁻¹ s⁻¹ [4], respectively, have been demonstrated in modulation-doped structures, which provide perfect material systems to study the physics of two dimensional hole/electron gases. To study the carrier transport in the HBT devices or in the two dimensional carrier gases, the carrier effective masses have to be determined. The hole effective masses of strained SiGe on Si have been reported by several workers, but some controversy is not yet resolved [5]. The effective mass of two dimensional elec-

trons in Si has been studied in the Si MOSFET [6] structures and in the strained-Si/relaxed-SiGe heterostructures [7]. However, to the best of our knowledge, there is no report of electron effective masses of SiGe in any structures.

The cyclotron resonance (CR) technique has been widely used to measure the electron effective masses in semiconductors. Because of the lack of high-quality bulk SiGe materials, we have to perform the CR measurements in SiGe epilayers on Si substrates. Owing to the small conduction band offset [8] between compressively strained SiGe and relaxed Si, electron confinement in strained-SiGe/relaxed-Si heterostructures is limited and CR cannot be performed. Theoretical calculations [8] and experimental results [3] showed that there was significant conduction band offset in tensilely strained-Si_{1-x}Ge_x/relaxed-Si_{1-y}Ge_y heterostructures as long as $x < y$. We have, therefore, fabricated such heterostructures by rapid thermal chemical vapor deposition (RTCVD) and investigated the electron effective masses in such structures.

2. Growth

All samples used in this study were grown by RTCVD. The growth system consists of a cold wall quartz tube with a loadlock. The wafer is supported on a quartz stand and heated by tungsten halogen lamps. The wafer temperature is accurately determined by monitoring infrared transmission through the wafer. The growth pressure is 6 Torr and the gases used are dichlorosilane (SiCl_2H_2) for silicon and germane mixture (0.8% GeH_4 in H_2) for germanium. The n-type doping is accomplished by adding phosphine mixture (70 ppm PH_3 in H_2) into the gas mixture. Details of the growth system can be found in Ref. [9]. The relaxed $\text{Si}_{0.62}\text{Ge}_{0.38}$ layers were grown on 100 mm lightly-doped p-type (100) Si wafers at 625°C after an initial high temperature (1000°C) cleaning in hydrogen. A compositionally graded buffer was used to reduce the threading dislocation density of relaxed $\text{Si}_{0.62}\text{Ge}_{0.38}$ layers. The Ge content of the buffer layer was graded from 0% at the Si substrate to 38% at the top of the graded layer over a distance of $\approx 0.5 \mu\text{m}$, and then a uniform $\text{Si}_{0.62}\text{Ge}_{0.38}$ layer with the thickness of $\approx 0.6 \mu\text{m}$ was deposited on the graded layer. Before the growth of active layers (electron channels), the structure was annealed in situ for 1 h at 800°C to ensure complete relaxation. X-ray diffraction shows the (400) SiGe peak of the 1 h annealed samples (800°C , in furnace with forming gas flow) shifts toward the (400) peak of Si substrate by 0.1° compared with the as-grown sample with the same buffers, but not annealed. No more shift is observed for the same sample annealed for another 9 h at 800°C . This indicates 1 h annealing time is sufficient at 800°C to relax the as-grown film completely. Modulation-doped structures were grown to confine electrons in the Si or $\text{Si}_{0.94}\text{Ge}_{0.06}$ channels. A $75 \text{ \AA}$ tensile strained Si or $\text{Si}_{0.94}\text{Ge}_{0.06}$ channel was grown on the buffer, followed by an undoped $100 \text{ \AA}$ $\text{Si}_{0.62}\text{Ge}_{0.38}$ relaxed spacer and a heavily phosphorus-doped $300 \text{ \AA}$ $\text{Si}_{0.62}\text{Ge}_{0.38}$ supply layer. The doping level in the supply layer was approximately $\approx 2 \times 10^{19} \text{ cm}^{-3}$, estimated by spreading resistance measurements. A schematic cross-section of the entire structure is shown in Fig. 1.

n^+ – $\text{Si}_{0.62}\text{Ge}_{0.38}$ cap $\sim 300 \text{ \AA}$	(relaxed)
i – $\text{Si}_{0.62}\text{Ge}_{0.38}$ spacer	(relaxed)
----- 2DEG -----	
i – $\text{Si}_{1-x}\text{Ge}_x$ channel $\sim 75 \text{ \AA}$	(strained)
in-situ annealed at 800°C for 1 hr	
uniform relaxed $\text{Si}_{0.62}\text{Ge}_{0.38}$	
$\sim 0.6 \mu\text{m}$	
graded SiGe buffer 0 – 38 % $\sim 0.5 \mu\text{m}$	
p-type Si substrate	

Fig. 1. Sample structures for effective mass measurements. The samples consist of $100 \text{ \AA}$ spacers, $\approx 2 \times 10^{19} \text{ cm}^{-3}$ n-type caps, and $\text{Si}_{1-x}\text{Ge}_x$ channels (0% or 6%) grown at 625°C .

Fig. 2. A plan-view TEM image of a relaxed buffer layer. A defect band clearly exists along the $\langle 110 \rangle$ direction.

The threading dislocation density was characterized by plan-view transmission electron microscope (TEM). The average separation between threading dislocations is about $5 \mu\text{m}$, indicating the threading dislocation density is around $4 \times 10^6 \text{ cm}^{-2}$. However, the threading defects are not distributed uniformly within the same sample, and 'defect bands' exist at the surface with a threading defect density of $\approx 10^8 \text{ cm}^{-2}$ (Fig. 2). The defect bands are aligned along the misfit dislocation directions, i.e. $\langle 110 \rangle$ directions. The origin of these defect bands is not clear at this point. The cross-sectional TEM (Fig. 3) shows that a dense network of misfit dislocations is confined in the graded buffers. Some dislocations penetrate deeply into the Si substrates. This is contradictory to Matthews and Blakeslee's theory [10], in which they assumed the dislocations were confined in the epilayers, because of relatively small thickness of the epilayers as compared to substrates. Similar results were also observed in the samples prepared by UHV (ultra high vacuum) CVD and a modified Frank–Read source [11] was proposed to explain this phenomenon. Relatively few dislocations terminated on the surface. The uppermost (active) layer appears largely dislocation free.

3. Cyclotron measurements

To measure the electron concentration and mobility, Hall measurements were carried out by using Van der Pauw geometry with Au:Sb contacts. A $50 \text{ \AA}$ Au layer, followed by $1500 \text{ \AA}$ Au:Sb alloys (0.6–24% Sb), and a $1000 \text{ \AA}$ Au layer was thermally evaporated and lifted off to form contact pads.

Fig. 3. A cross-sectional TEM image of a relaxed buffer layer. The dense network of dislocations is confined in the graded buffer layers and the top of uniform layer is relatively dislocation free. Some dislocations penetrate into the Si substrate.

Owing to the poor adhesion of Sb to the SiGe surface, the initial Au layer is crucial to avoid fall-off of the contact pads. Finally, the contacts were annealed at 350–400°C for 10–15 min to form ohmic contacts down to 10 K. Both samples showed typical modulation-doped behavior. The mobility increases monotonically for both samples with decreasing temperature, reaching 20 000 and 6420 $\text{cm}^2 \text{V}^{-1} \text{s}^{-1}$ at 10 K for Si and $\text{Si}_{0.94}\text{Ge}_{0.06}$ channels, respectively. The carrier density decreases with decreasing temperature and reaches 1.2×10^{12} and $1.4 \times 10^{12} \text{ cm}^{-2}$ at 10 K for Si and $\text{Si}_{0.94}\text{Ge}_{0.06}$ channels, respectively. Some parallel conduction was observed for the $\text{Si}_{0.94}\text{Ge}_{0.06}$ sample, but was removed after etching the supply layer. The magnetotransport experiments have been performed in similar structures and showed well-defined Shubnikov–de Hass oscillation in the longitudinal resistance and quantized Hall plateaux in the transverse resistance [12].

The Si and $\text{Si}_{0.94}\text{Ge}_{0.06}$ layers grown on relaxed $\text{Si}_{0.62}\text{Ge}_{0.38}$ buffers yield the tensile strain in the channels, which breaks the sixfold degeneracy in the bulk materials. The twofold conduction valleys along the growth direction is lower in energy than the fourfold conduction valleys perpendicular to the growth direction. At low temperature (4 K), the electrons in these two samples occupied the lowest valleys (confirmed by magnetotransport experiments [12]) and the effective mass measured in the two dimensional electron gas is the transverse electron mass (light mass). Fig. 4 shows the normalized transmission spectra ($T(B)/T(0)$) at 4 K with applied magnetic fields from 4 to 8 T for the two dimensional electron gas in the Si channel. The electron effective mass in Si can be determined by the slope of the plot of absorption peak frequency (in the unit of cm^{-1}) as a function of mag-

Fig. 4. Normalized cyclotron resonance spectra at 4 K of the Si channel with applied magnetic field from 4 to 8 T.

Fig. 5. Absorption peak frequency as a function of applied magnetic field for Si and $\text{Si}_{0.94}\text{Ge}_{0.06}$ channels. From the slopes, the effective masses of the two dimensional electron gases are determined.

netic field (Fig. 5), using $\omega_c = eB/m^*c$, where ω_c is the absorption frequency, e is the electron charge, B is the applied magnetic field, m^* is the effective mass, and c is the speed of light. The average effective mass is $0.203m_0$, slightly higher than that of the two dimensional electron gas in Si MOSFETs [6] ($0.198m_0$) with an electron concentration of $1 \times 10^{12} \text{ cm}^{-2}$ and that of Si/SiGe modulation-doped structures [7] ($0.195m_0$) with electron concentrations of $1.6\text{--}3.5 \times 10^{12} \text{ cm}^{-2}$. This might be due to the higher electron concentration in our sample, because previous studies [6,7] showed the electron effective mass of Si increases as the carrier concentration increases. Note that due to broad linewidth ($\approx 12 \text{ cm}^{-1}$), the estimated error bar is 5% in our experiments. It is possible that the slightly higher value of electron effective mass in our experiments is due to the uncertainty in the measurements.

The absorption spectra of the two dimensional electron gas in the $\text{Si}_{0.94}\text{Ge}_{0.06}$ channel are shown in Fig. 6 at 4 K with magnetic fields of 6 and 8 T. The effective mass of $\text{Si}_{0.94}\text{Ge}_{0.06}$ obtained from the plot of absorption peak as a function of applied field is $0.193m_0$. Compared to the absorption spectra

Fig. 6. Normalized cyclotron resonance spectra at 4 K of the $\text{Si}_{0.94}\text{Ge}_{0.06}$ channel with applied magnetic fields of 6 and 8 T. Compared with the absorption spectra of Si samples at 6 and 8 T (dotted line), the absorption spectra of $\text{Si}_{0.94}\text{Ge}_{0.06}$ consistently shift about 5% of the center frequency toward the high frequency side.

of Si samples at 6 and 8 T (Fig. 6), the absorption spectra of $\text{Si}_{0.94}\text{Ge}_{0.06}$ consistently shift about 5% of the center frequency toward high frequency side. Therefore, we conclude that electron effective mass ($0.193m_0$) of $\text{Si}_{0.94}\text{Ge}_{0.06}$ is about 5% lower than that of Si ($0.203m_0$), despite of the error bar of measurements. Two effects may be responsible to the lower electron effective mass of $\text{Si}_{0.94}\text{Ge}_{0.06}$: the different Ge content in the channels (0 versus 0.06) and the different strain (0.04×0.38 versus 0.04×0.32 , 0.04 is the misfit between Si and Ge) due to different lattice constant between the Si ($\text{Si}_{0.94}\text{Ge}_{0.06}$) channel and the $\text{Si}_{0.62}\text{Ge}_{0.38}$ relaxed buffer. Although the strain effect has been theoretically studied in some direct valleys [13], it is still not known in indirect conduction valleys. The change of effective mass solely due to the Ge content as in the bulk SiGe can not be determined.

4. Summary

We have successfully fabricated the strained $\text{Si}(\text{Si}_{0.94}\text{Ge}_{0.06})/\text{relaxed Si}_{0.62}\text{Ge}_{0.38}$ modulation-doped

structures with low threading dislocation densities and high electron densities in Si and $\text{Si}_{0.94}\text{Ge}_{0.06}$ channels. The cyclotron resonance measurements indicate the electron effective mass of strained $\text{Si}_{0.94}\text{Ge}_{0.06}$ on relaxed $\text{Si}_{0.62}\text{Ge}_{0.38}$ buffer is $0.193m_0$, which is about 5% lower than that of strained Si on the same buffer.

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References

- [1] E. Crabbe, B.S. Meyerson, J.M.C. Stork and D.L. Harame, *Tech. Dig. Int. Electron. Dev. Meet., IEEE, Piscataway, N.J., U.S.A.*, 1993, p. 83.
- [2] A. Schuppen, U. Erben, A. Gruhle, H. Kibble, H. Schumacher and U. König, *Tech. Dig. Int. Electron. Dev. Meet., IEEE, Piscataway, N.J., U.S.A.*, 1995, p. 743.
- [3] K. Ismail, M. Arafa, K.L. Saenger, J.O. Chu and B.S. Meyerson, *Appl. Phys. Lett.*, **66** (1995) 1077.
- [4] Y.H. Xie, Don Moroe, E.A. Fitzgerald, P.J. Silverman, F.A. Thiel and G.P. Watson, *Appl. Phys. Lett.*, **63** (1993) 2263.
- [5] T.E. Whall, A.D. Plews, N.L. Matthey and E.H.C. Parker, *Appl. Phys. Lett.*, **65** (1994) 3362.
- [6] J.P. Kotthaus, G. Abstreiter, J.F. Koch and R. Ranvaud, *Phys. Rev. Lett.*, **34** (1975) 151.
- [7] S.Q. Murphy, Z. Schlesinger, S.F. Nelson, J.O. Chu and B.S. Meyerson, *Appl. Phys. Lett.*, **63** (1993) 222.
- [8] C.G. van de Walle and R. Martin, *Phys. Rev. B*, **34** (1986) 5621.
- [9] J.C. Sturm, P.V. Schwartz, E.J. Prinz and H. Manoharan, *J. Vac. Sci. Technol. B*, **9** (1991) 2011.
- [10] J.W. Matthews and A.E. Blakeslee, *J. Cryst. Growth*, **27** (1974) 118.
- [11] F.K. LeGoues, B.S. Meyerson, J.F. Morar and P.D. Kirchner, *J. Appl. Phys.*, **71** (1992) 4230.
- [12] V. Venkataraman, C.W. Liu and J.C. Sturm, *J. Vac. Sci. Tech. B*, **11** (1993) 1176.
- [13] M. Jaffe and J. Singh, *J. Appl. Phys.*, **65** (1989) 329.