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Study of Quasi-Two Dimensional Hole Gas Si/Si_xGe_{1-x}/Si Quantum Wells

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Quasi-two-dimensional hole gas in strained Si/Si_xGe_{1-x}/Si quantum well structure is investigated both theoretically and experimentally. The hole effective mass and the charge distribution in the structure are achieved from the self-consistent solution of the Schrödinger-Poisson equations. High quality Si/$Si_{0.8}Ge_{0.2}$/Si p-type modulation doped quantum well has been grown by molecular beam epitaxy and the electrical properties have been measured. Hole mobility as high as $\sim$ 10400 cm^2/V with a sheet carrier concentration of $\sim 1.1 \times 10^{12}$ and the effective mass of $\sim 0.3m_0$ are obtained at T=4K.

1 INTRODUCTION

Recently P-type modulation doped Si/SiGe/Si quantum well structures have attracted great interest since they may be used to improve the properties of p-channel metal-oxide-semiconductor(PMOS) [1]. Shubnikov de Haas (SdH) and cyclotron measurements have recently used to determine the effective mass of carriers in the Si/SiGe/Si quantum well heterostructure [2, 3]. Although there have been several experimental reports on the electrical properties of modulation-doped p-type Si/SiGe/Si quantum well structures [2, 3], there remains clear comparision with rigorous theory, which can include strain, band mixing, and structural effects. Thus, Quasi-two-dimensional hole gas in strained Si/Si_xGe_{1-x}/Si quantum well structure is investigated both theoretically and experimentally in this paper.

2 SELFCONSISTENT FORMALISM

For general treatment of the valence bands, we use the Luttinger-Kohn(LK) Hamiltonian [4]. The application of an axial strain along the [001] growth direction will introduce additional terms in the Hamiltonian, the most important of which is the strain induced band edge splitting [5]. We solve the LK Hamiltonian as a numerical Finite-Difference(FD) eigenvalue problem, which yields the dispersion relation in the (k_x, k_y) plane. The potential profile in the growth direction of the device is determined by the self-consistent solution of the Schrödinger and Poisson equations [6].

Fig. 1 shows the SiGe/Si heterostructure, which was calculated and also grown by molecular beam epitaxy for experiments. The well is 200Å width and has two 50Å graded region at each interface. Two 5×10^{18} B-doped region is located on each side of the well and each has thickness of 50Å. The doped layers are separated from the well by spacer layers of 50Å.

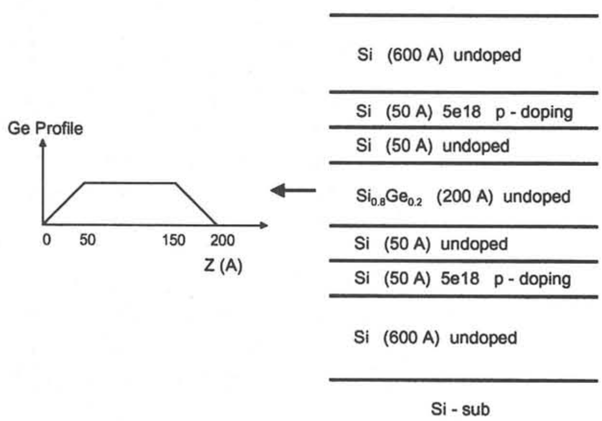

Fig. 1. The nominal SiGe/Si heterostructure.

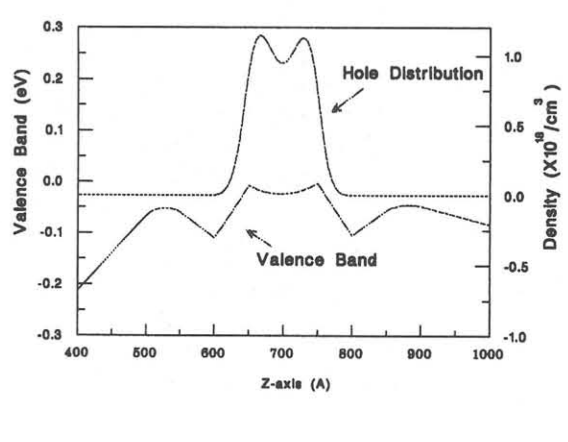

Fig. 2. Calculated valence band profile and hole distribution at T = 77K.

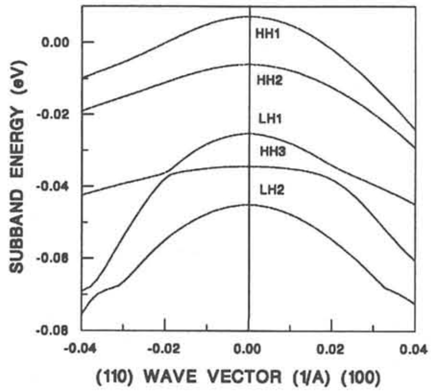

Fig. 3. Hole dispersion relation at T = 77K

Fig. 2 shows the valence band profile and hole distribution at 77K, and the associated hole subband dispersions are shown in fig. 3. Since the hole bands are nonparabolic, one must be careful to determine the hole effective mass. In order to average the masses for the hole states at a given temperature, one must know the hole distribution. Once the electron density is calculated with the real density of state, the effective mass can be obtained by

$$\int_0^\infty \frac{m^*}{\pi\hbar^2} f(E)dE = \int_0^\infty g(E)f(E)dE \qquad (1)$$

where $g(E)$ is the density of state calculated from the above E-k relations. The left hand side of eqn (1) includes the density of state with effective mass m*, which is to be found. At 300K, the effective hole mass of the first heavy hole subband is $0.43m_0$. Due to the fact that the hole subbands are highly nonparabolic, the averaged masses are strongly influenced by the temperature as well as doping density. This might explain the discrepancy between reported effective masses which are measured at different temperature and carrier densities. At lower temperature the carrier is squeezed closer to the tops of the bands. Since the mass at the top of the band is most light in the SiGe/Si QW, the averaged mass decreases with decreasing temperature. The averaged mass was calculated to be $0.249m_0$ at 77K. Table 1 shows the calculated results for the SiGe/Si heterostructure. This shows the effective hole mass of $0.20m_0$ and sheet charge density of $1.14\times10^{12}\text{cm}^{-2}$ at T = 4K. The above effective mass is similar to the recent reported experimental value [2]. It should be noted that the averaged masses of the structure are quite different at different temperatures.

3 EXPERIMENTS AND DISCUSSIONS

The $Si_{0.8}Ge_{0.2}$/Si modulation doped sample was grown by molecular beam epitaxy. This structure is given in fig. 1. Si sample which had the same doping profile without the quantum well also was grown for the comparison. These two samples are prepared for Hall measurement, velocity field measurement and SdH measurement. Ohmic contacts using Al were formed by alloying at 425 ^{o}C for 15 minutes.

Hall mobilities of the 2DHG were measured by utilizing a Van der Pauw structure. Measured Hall mobilities for SiGe/Si sample are shown in table 2 and compared with that of conventional p-MOSFET with inversion layer [7]. The hole mobility is 167 $\text{cm}^2/\text{V}\cdot\text{s}$ at 300K and increases to 991 $\text{cm}^2/\text{V}\cdot\text{s}$ at 77K. At the low temperature this value is a factor of 2 higher than previously reported Si p-MOSFET's.

The hole velocity of the SiGe/Si heterostructure was measured by means of pulsed current-voltage measurement [8]. The measured velocity - field($v-\varepsilon$) characteristics at 300K for the SiGe/Si heterostructure, compared with the Si sample are shown in fig. 4. The velocities of 6.6×10^5 and 4.7×10^5 cm/s are measured at E = 10 kV/cm for the SiGe/Si heterostructure and the Si sample, respectively. This value is lower than that of conventional bulk Si but in the same condition, the hole velocity of the SiGe/Si channel at the field is ~40% higher than that of the Si.

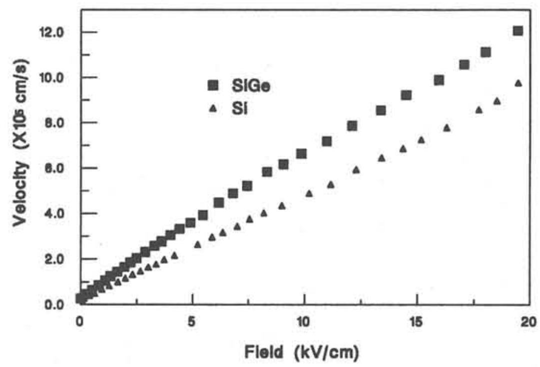

Fig. 4. Measured velocity field characteristics at 300K for the the SiGe/Si heterostructure, compared with those of Si sample.

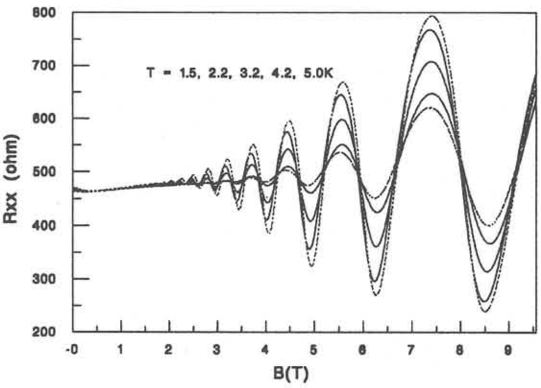

Fig. 5. Longitudinal resistance ρ_{xx} plotted vs. magnetic field B for a series of temperatures.

Also, we have carried out a detailed analysis of the temperature and magnetic field dependences of the magnetoresistance at temperatures down to 1.5K and in fields of up to 10 Tesla. The magnetic field dependence of longitudinal resistance (ρ_{xx}) has been measured in a sample of concentration x=0.2 and hole mobility mobility of 10,400

Channel	Subband No.	T = 300 n_s $\times 10^{12}$	m^*_{dos}	$E_n - E_f$ (meV)	State	T = 77 n_s $\times 10^{12}$	m^*_{dos}	$E_n - E_f$ (meV)	State	T = 4 n_s $\times 10^{12}$	m^*_{dos}	$E_n - E_f$ (meV)	State
SiGe	1	0.727	0.483	-52.5	HH1	0.957	0.249	7.3	HH1	1.086	0.200	13.1	HH1
	2	0.512	0.552	-66.3	HH2	0.296	0.333	-6.0	HH2	0.061	0.461	0.56	HH2
	3	0.241	0.545	-86.6	LH1	0.019	0.351	-25.2	LH1	0.		-17.1	LH1
	Total	1.783				1.278				1.147			

Table 1: The calculated results for $Si_{0.8}Ge_{0.2}/Si$ heterostructure

Sample No.	T = 300K μ_p ($cm^2/V \cdot sec$)	n_s ($\times 10^{12} cm^{-2}$)	T = 77K μ_p ($cm^2/V \cdot sec$)	n_s ($\times 10^{12} cm^{-2}$)
SiGe	167	7.56	991	1.57
Si	70	8.11	24	6.25
PMOS [7]	200		400	

Table 2: Hall measurement

$cm^2/v \cdot s$ is obtained at T=4K. Fig. 5 shows ρ_{xx} plotted against B at a series of temperature. A carrier sheet density of 1.07×10^{12} cm^{-2} is obtained from the period of ρ_{xx} vs. 1/B in low fields, and this is in good agreement with that from theoretical calculation. The amplitude of the oscillations can be described by [2],

$$\frac{\rho_{xx}}{\rho_0} = R_s V \frac{\xi}{\sinh \xi} \exp\left(-\frac{\pi}{w_c \tau_q}\right) \cos\left(\frac{2\pi E_f}{\hbar w_c}\right) \tag{2}$$

where

$$w_c = \frac{eB}{m^*}, \xi = \frac{2\pi^2 kT}{\hbar w_c}, E_f = \frac{\hbar^2 \pi N_s}{m^*}$$

for low field, where ρ_0 is the resistance at zero B, τ_q is the quamtum lifetime. Through the quantitative analysis, one can obtain a field independent value of $m^* = 0.30 m_0$. The effective mass differs from the theoretical one. This might be explained by that the grown structure has the narrower and/or shallower well than the norminal structure.

4 CONCLUSIONS

The valence band structure and the charge distribution in $Si/Si_xGe_{1-x}/Si$ structure are achieved from the self-consistent solution of the Schrödinger-Poisson equations. The theoretical calculation predicts the effective mass of $0.20 m_0$ at 4K, which are in fairly good agreement with expermental result. To characterize SiGe/Si channel experimentally, the SiGe/Si modulation doped samples for Hall, velocity vs. field, SdH measurement, were grown by molecular beam epitaxy. Our experimental results clearly show that strained p-type SiGe/Si channel has better transport properties than conventional p-MOSFET.

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