Hall mobility of narrow $\text{Si}_{0.2}\text{Ge}_{0.8}$ -Si quantum wells on $\text{Si}_{0.5}\text{Ge}_{0.5}$ relaxed buffer substrates

S. Tsujino,^{a)} C. V. Falub, E. Müller, M. Scheinert, and L. Diehl
Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, CH-5232 Villigen-PSI, Switzerland

U. Gennser
CNRS-LPN, F-91960 Marcoussis, France

T. Fromherz
Institut für Halbleiterphysik, Universität Linz, A-4040 Linz, Austria

A. Borak, H. Sigg, and D. Grützmacher
Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, CH-5232 Villigen-PSI, Switzerland

Y. Campidelli, O. Kermarrec, and D. Bensahel
STMicroelectronics, F-38926 Crolles-Cedex, France

(Received 23 September 2003; accepted 5 February 2004)

We studied in-plane transport of a two-dimensional hole gas in modulation-doped p - $\text{Si}_{0.2}\text{Ge}_{0.8}$ quantum wells (QWs) on $\text{Si}_{0.5}\text{Ge}_{0.5}$ relaxed buffer substrates with thicknesses L between 2.5 and 7 nm. We found that interface roughness scattering limits the low-temperature mobility μ of the samples with L between 2.5 and 4.5 nm. The interface roughness parameters were evaluated by fitting the experiment with the calculated μ limited by interface roughness scattering. We found that the obtained parameters were consistent with the values estimated from x-ray reflectivity and the transmission electron micrograph of the samples. When L is increased from 4.5 to 7 nm, μ increases only gradually and the highest μ of $0.44 \text{ m}^2/\text{Vs}$ was observed for 7-nm-thick QWs. The scattering by defects, interface charge, and strain fluctuation are discussed as possible additional mobility-limiting mechanisms. © 2004 American Institute of Physics. [DOI: 10.1063/1.1695102]

Ge-rich strained SiGe quantum wells prepared on virtual substrates have recently attracted attention for optoelectronic applications such as quantum cascade (QC) lasers.¹ When the Si-SiGe layers are strain symmetrized to the Ge concentration of the relaxed buffer virtual substrates, the growth of a large number of layers is possible while allowing large valence band offsets. These properties are suitable for Si-SiGe QC devices with sufficient optical gain. Our focus is on Si- $\text{Si}_{0.2}\text{Ge}_{0.8}$ strain symmetrized superlattice/quantum well (QW) structures prepared on $\text{Si}_{0.5}\text{Ge}_{0.5}$ relaxed buffer substrates. By employing the low-temperature solid source molecular beam epitaxy, we have demonstrated the growth of the highly planar QC structures containing layer thicknesses down to 0.4 nm and with the total thickness exceeding $1 \mu\text{m}$ giving a well-resolved mid-infrared electroluminescence signal.¹ In addition, we observed intersubband absorption,² and negative differential resistance in resonant tunneling superlattices³ and in double barrier diodes⁴ grown on these virtual substrates. Si-SiGe QWs with high-Ge concentration deposited on virtual substrates have also been studied intensively for the application to p -type metal-oxide-semiconductor field effect transistors.^{5,6}

In this work, we explore the low-temperature in-plane electrical transport of a two-dimensional hole gas in narrow $\text{Si}_{0.2}\text{Ge}_{0.8}$ QWs with various thicknesses, (2.5–7 nm). The low-temperature mobility indicates the scattering mechanism

relevant in the structures and the impact of the crystal quality on the electrical properties.

Here the samples are prepared by molecular beam epitaxy on (100) $\text{Si}_{0.5}\text{Ge}_{0.5}$ relaxed buffer substrates. The substrates are prepared by low-pressure chemical vapor phase deposition and subsequent chemical-mechanical polishing. We have adopted a low growth temperature of 330°C to kinematically limit the three-dimensional growth of the Ge-rich layers.⁷ Further details of the substrates and the growth procedure are described in Ref. 8. Each sample consists of four identical $\text{Si}_{0.2}\text{Ge}_{0.8}$ QWs with Si barriers separated by $\text{Si}_{0.5}\text{Ge}_{0.5}$ layers. The layer sequence of the samples is shown in Fig. 1. The thickness L of the QWs are, 2.5, 3.0, 3.5, 4.5, 5.5, and 7.0 nm. The thickness L_b of the Si barriers are 1.8 nm for the first four samples, 1.7 nm for the 5.5-nm-thick QW sample, and 2.1 nm for the 7.0-nm-thick QW sample. The separations between QW and the p -doped $\text{Si}_{0.5}\text{Ge}_{0.5}$ layers at both sides of QW are set to 6.8 nm by adjusting the $\text{Si}_{0.5}\text{Ge}_{0.5}$ spacer layer thickness. The p - $\text{Si}_{0.5}\text{Ge}_{0.5}$ layers are doped by boron atoms to $1 \times 10^{18} \text{ cm}^{-3}$. The cross section of the 3.0-nm-thick QW sample is examined by high resolution transmission electron microscopy (TEM) (Fig. 1 right). We found that all the interfaces are abrupt and undulations or structural degradations were negligible.

In the experiments, Hall mobilities and the hole concentrations were measured at various temperatures (Fig. 2). Measurements at temperatures higher than 80–150 K are difficult because of parallel conduction in the substrates of our samples. This parallel conduction freezes out below 80–150 K, but its influence is seen as an apparent steep variation of

^{a)}Electronic mail: soichiro.tsujino@psi.ch

FIG. 1. Layer sequence of quantum well samples (left) and high resolution transmission electron micrograph of a modulation doped Si-Si_{0.2}Ge_{0.8} quantum well sample (right), showing from the bottom to the top, Si_{0.5}Ge_{0.5} spacer, 1.8-nm-thick Si barrier, 3.0-nm-thick Si_{0.2}Ge_{0.8} quantum well, 1.8-nm-thick Si barrier, and Si_{0.5}Ge_{0.5} spacer layer. The direction of the growth is from the bottom to the top of the picture.

the hole concentration around the threshold temperature. However, below that temperature, the hole concentration is approximately constant, nominally $1 \times 10^{16} \text{ m}^{-2}$ per QW. The exact two-dimensional hole concentration at low temperature and the threshold temperature vary between samples because of doping fluctuations. Figure 2(b) shows that the mobility decreases as the temperature is increased for all the QWs except the two narrowest samples. The decrease became slightly steeper above ~ 60 K. For the 2.5-nm-thick QW sample, the mobility increases up to a temperature of 60 K.

Figure 3 summarizes the mobility μ at 8 K as a function of QW thickness L . The highest μ of $0.44 \text{ m}^2/\text{Vs}$ obtained for the 7-nm-thick sample at 8 K is larger than the recently reported value of $0.062 \text{ m}^2/\text{Vs}$ for a 10-nm-thick Si_{0.2}Ge_{0.8} QW grown at 300°C on Si_{0.8}Ge_{0.3} virtual substrates.⁹ The factor 7 higher mobility of our sample reflects the small roughness of the substrates and the small thickness fluctuation of our samples. When L is increased from 2.5 to 4.5 nm, μ increases steeply. In this range, we find that the slope is given by $(\partial E_{\text{HH},1}/\partial L)^{-2}$, indicating that μ is limited by the interface roughness scattering,¹⁰ where $E_{\text{HH},1}$ is the quantized energy of the lowest heavy-hole subband (HH₁). When L exceeds 4.5 nm, μ only increases gradually.

FIG. 2. Results of Hall measurements of the Si_{0.2}Ge_{0.8}-Si quantum well samples at various temperatures, showing the hole concentrations p divided by the number of QWs (a) and the Hall mobility μ (b).

FIG. 3. The relation between the low-temperature mobility of Si_{0.2}Ge_{0.8}-Si QWs and the quantum well thickness, for the as-grown samples (closed squares) and annealed samples (open squares). The solid curve (μ_{IFR}) shows the mobility limited by interface roughness scattering calculated with the average roughness height $\Delta = 0.4 \text{ nm}$ and the correlation length $\Lambda = 2.3 \text{ nm}$. Also shown are the calculated mobilities limited by remote ionized impurity scattering (μ_{imp}), by alloy disorder scattering (μ_{alloy}), by interface charge scattering with charge density $0.25 \times 10^{16} \text{ m}^{-2}$ per interface ($\mu_{\text{if-charge}}$), and by strain fluctuation by the interface roughness with two different models ($\mu_{\text{strain,QW}}$ and $\mu_{\text{strain,B+QW}}$).

First we discuss the mobility below 4.5 nm. To analyze the L dependence of μ quantitatively, we calculated the momentum relaxation time τ and the mobility $\mu = e\tau/m^*$ by standard transport theory,¹¹ where m^* is the in-plane effective mass in the QWs. We assumed a parabolic dispersion for HH₁ with $m^* = (0.16 \pm 0.2)m_0$, based on the $k \cdot p$ calculation for our samples, where m_0 is the free electron mass. The vertical effective mass and the valence band offsets of our QWs are evaluated following the method of Refs. 12 and 13. These values reproduced the energy separation between HH₁ and the first excited heavy hole subband (HH₂) observed by the intersubband optical absorption.² We also assumed that carriers occupy only HH₁ because the energy separation to the excited subbands is more than $\sim 80 \text{ meV}$, which is larger than the estimated Fermi energy (12–24 meV) in our samples. The averaged potential of the interface roughness scattering with the gaussian correlation is given by $V(\mathbf{q})^2 = \pi \Delta^2 \Lambda^2 (\partial E_{\text{HH},1}/\partial L)^2 \exp(-\Lambda^2 \mathbf{q}^2/4)$, where Δ is the average roughness height and Λ is the correlation length.¹⁰ Assuming that the bottom and the top barrier-QW interfaces are uncorrelated, the calculated scattering rate has to be multiplied by 2 at the end. We use the value of Δ equal to 0.4 nm evaluated from the TEM cross section of the samples and fit the experiment with Λ .

We find that the mobility of the samples below 4.5 nm is well reproduced with the values, $\Delta = 0.4 \text{ nm}$ with $m^* = (0.16 \pm 0.2)m_0$ and $\Lambda = 2.3 \pm 0.3 \text{ nm}$ (the curve μ_{IFR} in Fig. 3). The fitting error is equal to $\pm 10\%$. These roughness parameters are consistent with the values obtained from the

analysis of x-ray reflectivity, Δ equal to 0.4–1.5 nm and Λ equal to 2.0 ± 0.5 nm for the strain symmetrized Si–SiGe superlattices deposited using the same conditions.¹⁴ We note that the calculated μ is in fact a two-valued function of Λ and it is possible to fit the mobility using Λ equal to 8.1 ∓ 0.5 nm. However, from the x-ray reflectivity and the cross-sectional TEM, we conclude that Λ equal to 2.3 ∓ 0.3 nm is appropriate for our samples.

The rapid decrease of the effect of the roughness above 5 nm suggests that other scattering processes take effect for these samples. Our calculations show that the scattering by remote ionized impurities and the alloy disorder limits the mobility at around $10 \text{ m}^2/\text{Vs}$ (μ_{imp} and μ_{alloy} in Fig. 3, respectively) and not important in our samples. Defects such as threading dislocations¹⁵ and/or point defects can have an influence. The effect of dislocations is likely to be small here because QWs are below the Matthews–Blakeslee critical thickness,¹⁵ and also because the mean separation, larger than $\sim 1 \mu\text{m}$, between dislocations in the epi-layer is much larger than the estimated mean free path of ~ 80 nm for the highest mobility sample. However, point defects can be important because the creation of the lattice vacancies and/or the incorporation of the background impurities are enhanced at the low growth temperature.

In the case of bulk Si, the density of lattice vacancies is decreased by annealing at moderate temperature $\sim 600^\circ\text{C}$.¹⁶ We found that the samples annealed at 600°C for 15 min in forming gas (1% H_2 diluted by N_2) show a slight increase of μ at 8 K: from $0.34 \text{ m}^2/\text{Vs}$ for as grown sample to $0.38 \text{ m}^2/\text{Vs}$ after annealing, and from 0.44 to $0.49 \text{ m}^2/\text{Vs}$ for samples containing 5.5-nm-thick QWs and the 7-nm-thick quantum wells, respectively. The annealing did not change the hole concentrations or the temperature dependence of the mobility. The results were the same for the samples annealed at the same temperature but for 30 min. Here we chose the annealing condition not to influence the layer structures by the intermixing/diffusion of Ge atoms. This assumption is verified by comparing photoluminescence, intersubband absorption, as well as x-ray diffraction measurements before and after the annealing. Comparing with the annealing effect of bulk Si,¹⁶ the $\sim 10\%$ increase of the mobility is ascribed to the decrease of the vacancy-like defects by the annealing, however, the density of the remaining point defects are still unknown.

We further consider two other scattering mechanisms, the strain fluctuation^{17,18} and the interface charge.¹⁹ Since the interface charge density in our samples is unknown, we used $0.25 \times 10^{16} \text{ m}^{-2}$ per interface ($0.5 \times 10^{16} \text{ m}^{-2}$ in total), taking the average of the reported value $(0.1\text{--}0.4) \times 10^{16} \text{ m}^{-2}$ for $\text{Si}_{0.8}\text{Ge}_{0.2}$ –Si interface.¹⁹ The calculated mobility ($\mu_{\text{if-charge}}$ in Fig. 3) has a value of $2 \text{ m}^2/\text{Vs}$ at 7 nm showing the importance of this mechanism. The strain fluctuation here is induced by the interface roughness giving rise to a scattering potential proportional to $f\Xi_u\Delta$ confined within k_F^{-1} around the interface, where f is the lateral strain of the struc-

ture, Ξ_u is the deformation potential constant, and k_F^{-1} is the Fermi wavelength of the samples equal to 3–4.8 nm. We adopted the potential given in Ref. 19 to our QWs and calculated μ with two models as shown in Fig. 3. $\mu_{\text{strain,QW}}$ is calculated using f equal to the strain $f_{\text{QW}} = 0.01$ of QW, while $\mu_{\text{strain,B+QW}}$ is calculated using f equal to the summation $(|f_{\text{QW}}| + |f_B|)$ where f_B is the strain of the barrier. Since the Si barrier is also strained, f_B should also contribute to the strain fluctuation. However, since the Si-barrier thickness is smaller than k_F^{-1} , it is likely that the effect is weakened and that $\mu_{\text{strain,QW}}$ and $\mu_{\text{strain,B+QW}}$ give the approximate boundary for the strain fluctuation limited mobility in our samples. These results suggest that both mechanisms are important. However, for a quantitative explanation, further study is required to determine the amount of the interface charge, and the distribution of the strain.

The authors acknowledge A. Weber and D. Bächli for their help on device processing, S. Stutz for technical help on the electrical measurement system, and J. Gobrecht for the critical reading of the manuscript. The work has been partially supported by Swiss National Foundation and the European community within the SiGeNET project and the SHINE project.

¹L. Diehl, S. Mentese, H. Sigg, D. Grützmacher, E. Müller, U. Gennser, I. Sagnes, Y. Campidelli, O. Kermarrec, D. Bensahel, and J. Faist, *Appl. Phys. Lett.* **81**, 4700 (2002).

²L. Diehl, H. Sigg, G. Dehlinger, D. Grützmacher, E. Müller, U. Gennser, I. Sagnes, T. Fromherz, Y. Campidelli, O. Kermarrec, D. Bensahel, and J. Faist, *Appl. Phys. Lett.* **80**, 3274 (2002).

³S. Tsujino, S. Mentese, L. Diehl, E. Müller, B. Haas, D. Bächle, S. Stutz, D. Grützmacher, Y. Campidelli, O. Kermarrec, and D. Bensahel, *Appl. Surf. Sci.* **224**, 377 (2004).

⁴U. Gennser *et al.* (unpublished).

⁵F. Schäffler, *Semicond. Sci. Technol.* **12**, 1515 (1997).

⁶T. E. Whall, *J. Cryst. Growth* **157**, 353 (1995).

⁷R. L. Headrick and J.-M. Baribeau, *J. Vac. Sci. Technol. A* **13**, 782 (1995).

⁸D. Grützmacher, S. Mentese, E. Müller, L. Diehl, H. Sigg, Y. Campidelli, O. Kermarrec, D. Bensahel, T. Roch, J. Stangl, and G. Bauer, *J. Cryst. Growth* **251**, 707 (2003).

⁹M. Myronov, P. J. Phillips, T. E. Whall, and E. H. C. Parker, *Appl. Phys. Lett.* **80**, 3557 (2002).

¹⁰H. Sakaki, T. Noda, K. Hirakawa, M. Tanaka, and T. Matsusue, *Appl. Phys. Lett.* **51**, 1934 (1987).

¹¹See, e.g., A. Gold, *Phys. Rev. B* **38**, 10798 (1988); V. Senz, T. Ihn, T. Heinzel, K. Ensslin, G. Dehlinger, D. Grützmacher, U. Gennser, E. H. Hwang, and S. Das Sarma, *Physica E* **13**, 723 (2002).

¹²C. G. Van de Walle, *Phys. Rev. B* **39**, 1871 (1989).

¹³R. Winkler, M. Merkler, T. Dahnhofer, and U. Rössler, *Phys. Rev. B* **53**, 10858 (1996).

¹⁴M. Meduna, J. Novak, G. Bauer, V. Holy, C. V. Claudiu, E. Müller, S. Tsujino, D. Grützmacher, Y. Campidelli, O. Kermarrec, and D. Bensahel, *Z. Kristallogr.* (in press).

¹⁵K. Ismail, F. K. LeGoues, K. L. Saenger, M. Arafat, J. O. Chu, P. M. Mooney, and B. S. Meyerson, *Phys. Rev. Lett.* **73**, 3447 (1994).

¹⁶H.-J. Gossmann, P. Asoka-Kumar, T. C. Leung, B. Nielsen, K. G. Lynn, F. C. Unterwald, and L. C. Feldman, *Appl. Phys. Lett.* **61**, 540 (1992).

¹⁷R. M. Feenstra and M. A. Lutz, *J. Appl. Phys.* **78**, 6091 (1995).

¹⁸R. J. P. Lander, M. J. Kearney, A. I. Horrell, E. H. C. Parker, P. J. Phillips, and T. E. Whall, *Semicond. Sci. Technol.* **12**, 1064 (1997).

¹⁹C. J. Emeleus, T. E. Whall, D. W. Smith, R. A. Kubiak, H. C. Parker, and M. J. Kearney, *J. Appl. Phys.* **73**, 3852 (1993).