Photocurrent and transmission spectroscopy of direct-gap interband transitions in Ge/SiGe quantum wells

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The authors studied the direct-gap interband transitions in strain-compensated Ge/SiGe quantum wells grown by low energy plasma enhanced chemical vapor deposition. A series of excitonic interband absorptions from the quantized hole states to the quantized electronic states at the Γ_{7c}^- edge in the Ge wells is observed up to room temperature by photocurrent and transmission spectroscopy. The results are compared with theory. At low temperature, the quantum confined Stark effect is demonstrated in a Schottky diode geometry. © 2006 American Institute of Physics.

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Development of optoelectronic devices such as efficient light sources and optical modulators compatible with Si-processing technology is the key to the implementation of optical interconnects in Si-integrated circuits.^{1,2} The indirect nature of the fundamental interband transitions has limited the use of the interband transitions in Si including SiGe alloys. Existing Si light modulators employ weak effects and therefore require relatively long waveguides^{3,4} or resonant enhancement in a high-quality-factor cavity.⁵ However, the use of the direct-gap interband transitions between the Γ_{8v}^+ edge and the Γ_{7c}^- edge in SiGe heterostructures, or E_0 transitions, has the potential to realize broadband optical modulators with micrometer size.¹ Since the E_0 transition energy increases rapidly with the decrease of the Ge content of SiGe alloy, the Γ_{7c}^- -electronic states in Ge layers are quantum mechanically confined by SiGe layers. In such a Ge/SiGe heterostructure prepared by reduced-pressure chemical vapor deposition, Kuo *et al.* have recently demonstrated the $\Gamma_{8v}^+ - \Gamma_{7c}^-$ excitonic interband transition and the quantum confined Stark effect at room temperature by photocurrent spectroscopy.⁶ Here we present a detailed comparison of the transition energies detected by photocurrent and transmission and of the measured absorption spectrum with theory. A good agreement between observed and calculated peak positions is obtained. In addition, upon application of an electric field by a Schottky electrode at low temperature, a quadratic shift of the absorption edge is observed which demonstrates the quantum confined Stark effect.

The sample consists of ten periods of 12-nm-thick Ge quantum wells sandwiched by 24-nm-thick $\text{Si}_{0.15}\text{Ge}_{0.85}$ barriers on a $\text{Si}_{0.1}\text{Ge}_{0.9}$ relaxed buffer deposited by low energy plasma enhanced chemical vapor deposition (LEPECVD).⁷ On a Si (100) substrate, first a graded $\text{Si}_{1-y}\text{Ge}_y$ buffer is deposited with the growth rate of 5–10 nm/s at a substrate temperature decreasing from 750 to 560 °C with increasing Ge content. The Ge content y of the buffer is linearly graded at a rate of 7 % / μm starting with y equal to 0. After reaching the final value of y equal to 0.9, 2 μm of $\text{Si}_{0.1}\text{Ge}_{0.9}$ is deposited on top of the graded layer. Thereon, a 400-nm-thick p^+

$\text{Si}_{0.1}\text{Ge}_{0.9}$ bottom contact, a 50-nm-thick $\text{Si}_{0.1}\text{Ge}_{0.9}$ spacer, the ten periods of the Ge quantum well structure, and a 50-nm-thick $\text{Si}_{0.1}\text{Ge}_{0.9}$ cap layer are deposited at 0.4 nm/s at 520 °C. We note that the topmost $\text{Si}_{0.1}\text{Ge}_{0.9}$ buffer layer is fully relaxed without additional annealing. This is shown by x-ray diffraction measurements of the sample in the (004) and the (224) directions.

The photocurrent and the transmission spectrum of the sample are measured by Fourier transform infrared spectroscopy. For the photocurrent measurement, the sample is processed into a square-shaped mesa diode having $0.9 \times 0.9 \text{ mm}^2$ area. 10 nm of Cr is deposited on top of the mesa which serves as a semitransparent Schottky gate electrode. An Ohmic contact to the bottom $p^+ \text{Si}_{0.1}\text{Ge}_{0.9}$ contact layer is achieved by depositing 200 nm of Al on top of the $p^+ \text{Si}_{0.1}\text{Ge}_{0.9}$ layer exposed by reactive ion etching (RIE). The reference for the photocurrent is obtained by measuring the transmission function of the system with a pyroelectric detector with flat optical response. The transmission spectra T_s are measured for an unprocessed sample with mirror-polished back side using a liquid-nitrogen cooled mercury cadmium telluride detector. For reference, a sample without quantum well layers is prepared by removing the top layers by RIE. The data are presented in absorbance unit, $-\log_{10}(T_s/T_{\text{ref}})$, where T_{ref} is the respective reference spectrum.

Figure 1 shows the photocurrent spectrum of the sample measured at 17 K when the bias voltage is equal to 0 V. We observed a series of steps above 0.97 eV, which is ~ 0.2 eV above the indirect fundamental band gap of Ge. In addition, the onset of steps is decorated by a peak structure indicating an excitonic effect. Figure 2 shows the band diagram and calculated hole and electron wave functions of the Ge quantum well at the Γ edge. The quantized hole states are calculated by the six-band $\mathbf{k} \cdot \mathbf{p}$ method.⁸ The strain and Ge-concentration dependent conduction band energies are calculated by using parameters described in Refs. 9 and 10. The lowest conduction band states are located in the L valley. Its conduction band edge is shown in Fig. 2(a) by a broken line. The Γ_{7c}^- edge of the Ge well layer is confined by that of the $\text{Si}_{0.15}\text{Ge}_{0.85}$ layers with a band offset of ~ 0.3 eV. Assum-

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FIG. 1. (Color online) Photocurrent responsivity of Ge quantum wells prepared on a $\text{Si}_{0.1}\text{Ge}_{0.9}$ virtual substrate measured at 17 K with bias equal to 0 V. The lower curve shows the calculated interband absorption spectrum for light polarization along the quantum well plane. The arrows indicate the onset of the quantized E_0 transitions in the quantum well between confined hole states and confined electronic states at the Γ_{7c}^- edge. The broken lines show the onset of the corresponding transitions for the calculated spectrum. The absence of the peak structure at the absorption edge of the calculated $\text{HH}_1\text{-}E_1$ transition indicates that the observed $\text{HH}_1\text{-}E_1$ peak is due to the exciton effect.

ing the effective mass m^* equal to $0.04m_0$,¹¹ the lowest Γ_{7c}^- electronic states are calculated, as shown in Fig. 2. From symmetry, we expect to observe the interband transition series consisting of $\text{HH}_1\text{-}E_1$, $\text{LH}_1\text{-}E_1$, $\text{HH}_2\text{-}E_2$, $\text{LH}_2\text{-}E_2$, etc., where HH_n , LH_n , and E_n denote the n th heavy hole, light hole, and electron states, respectively. We find that the calculated $\text{HH}_1\text{-}E_1$ transition energy is equal to 0.977 eV in good agreement with the lowest peak position at 0.978 eV observed in the experiment. For better comparison, we calculated the interband absorption spectrum for light polarization along the well. First, the absorption $\alpha_k(\omega)$ associated with the generation of an electron-hole pair in the Ge quantum well at in-plane wave vector $\mathbf{k}$ is calculated using a constant interband matrix element of the velocity operator, applying the known selection rules¹² and assuming 3 meV broadening. After summing up the contributions from electron-hole pairs having their transition energies below 1.5 eV and integrating over $\mathbf{k}$, the spectrum shown in Fig. 1 (lower curve) is obtained. The good overall agreement between theory and experiment confirms the peak assignment for photon energies below ~ 1.2 eV.

Above ~ 1.3 eV the calculation predicts that the absorption monotonically increases reflecting the onset of the absorption by transitions between HH and LH continuum states and the continuum Γ_{7c}^- electron states, Fig. 2(a). This increase is observed in the experiment. The peak at 1.224 eV observed in the experiment is absent in the calculation. We ascribe this to the E_0 transition taking place in the $\text{Si}_{0.1}\text{Ge}_{0.9}$ spacer and cap layer. The expected onset energy of 1.213 eV is in close agreement with the experiment.

The peak structure observed at the onset of the transitions is in part ascribed to the highly nonparabolic dispersion of hole states due to the intravalence band mixing. The calculated hole subbands in Fig. 2(b) show that, in the case of the HH_2 subband, the dispersion is nearly flat around $\mathbf{k}$ equal to 0. This results in the increase of the joint density of states of the $\text{HH}_2\text{-}E_2$ transition and leads to an enhanced absorption near the onset, as shown in the bottom curve of Fig. 1. The enhancement of the calculated $\text{LH}_1\text{-}E_1$ absorption edge is

FIG. 2. (Color online) (a) Energy band diagram of a Ge quantum well on a $\text{Si}_{0.1}\text{Ge}_{0.9}$ virtual substrate at the Γ edge and (b) in-plane subband dispersion of the hole states along the [100] direction (solid curves) and along the [110] direction (dotted curves). The hole states are calculated by a six-band $\mathbf{k}\cdot\mathbf{p}$ method. The electron states are calculated with strain-dependent band-gap parameters assuming a constant effective mass. The zero of the energy is chosen as the valence-band edge of the unstrained $\text{Si}_{0.1}\text{Ge}_{0.9}$ layer.

less pronounced but still visible. For the HH_1 state, however, the mixing effect is much weaker. Consequently, no enhancement is predicted for the calculated $\text{HH}_1\text{-}E_1$ absorption edge. Therefore, the $\text{HH}_1\text{-}E_1$ peak observed in the experiment is unambiguously ascribed to the exciton effect. In contrast to high-purity bulk Ge,⁸ excitonic transitions are not separated from the interband continuum in our sample, which we ascribe to the linewidth broadening due to intervalley scattering, interface roughness, and inhomogeneities of the sample. We found that the half-width broadening of the $\text{HH}_1\text{-}E_1$ exciton transition evaluated from the lower energy tail is equal to 6 meV, which conforms to the intervalley scattering lifetime of ~ 100 fs measured at low temperatures.¹³ To compare with this value, we evaluated the upper bound of the expected binding energy E_B^* of the $\text{HH}_1\text{-}E_1$ exciton by referring to the result of the variational calculation in Ref. 14 using the electron mass equal to $0.04m_0$ and the calculated band edge effective mass of the HH_1 state equal to $0.08m_0$. We found that E_B^* is equal to 3.9 meV which is indeed smaller than the observed broadening.

Figure 3(a) shows photocurrent spectra at 17 K for reverse bias from zero up to 0.8 V. We found that the $\text{HH}_1\text{-}E_1$ excitonic peak gradually disappears with increase of the bias. Similarly, the peak at the onset of the $\text{LH}_1\text{-}E_1$ peak and the $\text{HH}_2\text{-}E_2$ peak diminishes with bias, but the peak structure remains up to 0.8 V. This observation again suggests the importance of nonparabolic dispersion for these states. At about -0.1 V, shown in Fig. 3(b), the photocurrent disappears indicating the flatband condition. Below -0.1 V, the signal changes sign. Figure 3(c) shows the relation between the bias and the $\text{HH}_1\text{-}E_1$ absorption edge taken at half-maximum. We found that the shift of the $\text{HH}_1\text{-}E_1$ transition varies quadratically with bias, consistent with the quantum confined Stark effect.¹⁵

Figure 4 shows the photocurrent spectrum PC and the absorption spectra A obtained by a transmission measurement at higher temperatures. When the sample temperature is increased, all the observed peaks shift to lower photon en-

FIG. 3. (Color online) (a) Low-temperature photocurrent responsivity spectra obtained at reverse biases of 0, 0.2, 0.4, 0.6, and 0.8 V. Bias dependence of the photocurrent at selected energies (b) and the HH_1-E_1 absorption edge at the half-maximum (c) are also shown. The flatband condition is reached at the bias equal to ~ -0.1 V. The curve in (c) shows a parabolic fit centered at -0.1 V.

ergy. This temperature-induced shift agrees with the expected temperature dependence of the direct band gap of Ge.¹⁶ At 160 K, the HH_1-E_1 peak coincides with $1.31 \mu\text{m}$. When the temperature is increased from 20 to 200 K, we found that the broadening of the HH_1-E_1 excitonic transition (half-width at half-maximum) increases from 6 to 12 meV linearly with temperature, indicating the decreasing lifetime of the E_1 state at higher temperatures. At room temperature, the photocurrent measurement was difficult due to the increased leakage current. However, the transmission spectrum in Fig. 4 clearly shows that the HH_1-E_1 transition is still excitonic at room temperature. From the absorption spectrum, we found that the absorption strength of the HH_1-E_1 transition is equal to $(3.1 \pm 0.1) \times 10^{-3}$ which corresponds to $(0.70 \pm 0.02)\%$ per well. This value is comparable to the interband absorption strength of two-dimensional carriers in III-V semiconductors.¹⁷ The absorption coefficient as defined by the thickness of the Ge well is equal to $\sim 5000 \text{ cm}^{-1}$, which is $\sim 30\%$ larger than for the direct-gap excitonic absorption of bulk Ge.

In summary, we have observed the direct-gap interband excitonic absorption of strain-compensated $\text{Ge}/\text{Si}_{0.15}\text{Ge}_{0.85}$ multiple quantum wells on a $\text{Si}_{0.1}\text{Ge}_{0.9}$ relaxed buffer grown by the LEPECVD method. We found a reasonable agreement for the calculated energies with the observed peak positions. By comparing to the calculated absorption spectrum, the observed peak structures at the transition onsets are ascribed to the exciton effect and/or band nonparabolicity in the valence band. At low temperature, we observed the quantum confined Stark effect in a Schottky diode configuration. We de-

FIG. 4. (Color online) Photocurrent responsivity spectrum PC at zero bias at 160 K and absorption spectra A measured at 160 and 300 K.

termined the absorption strength of 0.7% per well with a transmission measurement.

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