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Research Article

Photoreflectance Spectroscopy Characterization of $Ge/Si_{0.16}Ge_{0.84}$ Multiple Quantum Wells on Ge Virtual Substrate

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We report a detailed characterization of a $Ge/Si_{0.16}Ge_{0.84}$ multiple quantum well (MQW) structure on Ge-on-Si virtual substrate (VS) grown by ultrahigh vacuum chemical vapor deposition by using temperature-dependent photoreflectance (PR) in the temperature range from 10 to 300 K. The PR spectra revealed a wide range of optical transitions from the MQW region as well as transitions corresponding to the light-hole and heavy-hole splitting energies of Ge-on-Si VS. A detailed comparison of PR spectral line shape fits and theoretical calculation led to the identification of various quantum-confined interband transitions. The temperature-dependent PR spectra of $Ge/Si_{0.16}Ge_{0.84}$ MQW were analyzed using Varshni and Bose-Einstein expressions. The parameters that describe the temperature variations of various quantum-confined interband transition energies were evaluated and discussed.

1. Introduction

Semiconductor quantum well heterostructures have been implemented in many commercial optoelectronic devices. Definitely Si-based light emitting source integration is one of the most attractive candidates for photonic integration [1, 2]. Kuo et al. first reported the strong quantum-confined Stark effect (QCSE) in Ge/SiGe multiple quantum well (MQW) structure grown on Si substrate [3]. The high speed optoelectronic devices such as optical modulators based on QCSE [4, 5] and photo detectors [6, 7] are also realized. Recently, the direct gap room temperature photoluminescence properties of Ge MQWs [8] and the observation of above room temperature photoluminescence in Ge/SiGe MQWs structure were investigated [9]. The electroluminescence properties of the material system emitting in 1.55 μm region for optical telecommunication have also been reported [10, 11]. These results showed that Ge/SiGe MQW can be a promising candidate for efficient light emitting devices for Si-based photonic circuits. Note that at room temperature, the direct gap of Ge at the Γ point is only 140 meV above the indirect fundamental gap [12]. Previous study reported tensile strained Ge/SiGe MQW [13], which may be exploited to cover the range of wavelengths used in telecommunications and for longer wavelength applications in health care and pollution monitoring devices [14]. However, with different growth conditions, compressively strained Ge/SiGe MQW on virtual substrate (VS) has been grown and confirmed by photocurrent [15], photoreflectance (PR) [16], and piezoreflectance spectroscopies [17, 18] studies. The existence of compressive strain in Ge/SiGe MQW structure during growth would increase the energy gap which is not beneficial for long wavelength applications. A detailed investigation of the material system may provide useful information for crystal growers, so that optimal growth conditions can be set to fabricate desirable tensile strained Ge/SiGe MQW.

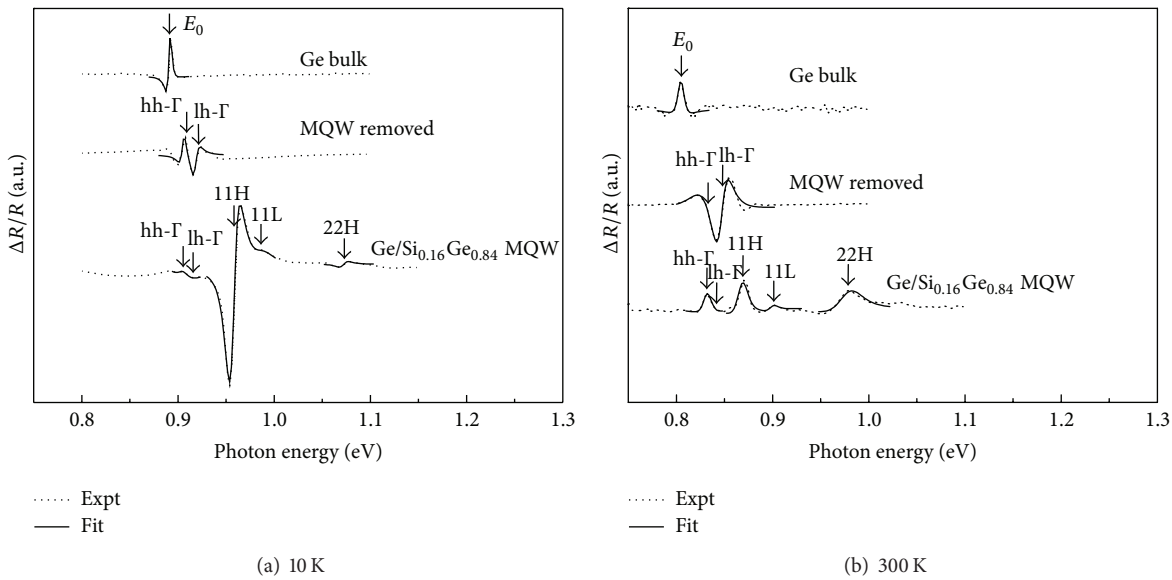


Figure 1: The experimental PR spectra (dashed curves) of Ge bulk, MQW removed sample, and Ge/Si$_{0.16}$Ge$_{0.84}$ MQW structure at (a) 10 K and (b) 300 K. The solid lines are fit to the first derivative of Lorentzian line-shape functional form. The obtained various transition energies are indicated by the arrows.

In this study, we present a detailed study of a Ge/Si$_{0.16}$Ge$_{0.84}$ MQW structure grown on Ge-on-Si VS by temperature-dependent PR measurements in the range between 10 and 300 K. The Ge/Si$_{0.16}$Ge$_{0.84}$ MQWs structures were grown by ultrahigh vacuum chemical vapor deposition [19]. The PR spectra of Ge/Si$_{0.16}$Ge$_{0.84}$ MQW structure displayed a series of features originating from quantum-confined interband transitions as well as the splitted band-gap energies of the Ge-on-Si VS. A comprehensive analysis of PR spectra and comparison with theoretical calculation led to the identification of various quantum-confined interband transitions. In addition, the parameters that describe the temperature dependence of the transition energies were evaluated. The use of PR as a nondestructive optical characterization technique for Ge/SiGe MQW was demonstrated.

2. Experimental

The samples were grown on 10 cm diameter n-type (001) Si wafers with a resistivity of 0.1–1.2 Ω-cm by a cold-wall ultrahigh vacuum chemical vapor deposition system with a base pressure of 3×10^{-10} Torr. After thermal cleaning of the Si substrate at 850°C for 30 min, a 300 nm thick Si buffer layer was grown at 750°C. The growth of the structures was divided into two steps. The first part of the structure was a Ge-VS, including a 90 nm low temperature Ge seed layer and 340 nm high-temperature Ge layer. Six periods of Ge/SiGe MQW were then grown on Ge-on-Si VS at 600°C with a Ge mole fraction of 0.84 in the SiGe barriers. The thickness of well (11 nm) and barrier (26 nm) was estimated by double crystal X-ray diffraction measurements.

For PR measurement, the modulation of built-in electric field was caused by photoexcited electron-hole pairs created by a mechanically chopped 532 nm line (~10 mW) of a laser diode with modulating frequency at ~200 Hz. The radiation from a 150 W tungsten-halogen lamp dispersed by a 0.25 m monochromator provided the monochromatic light. The reflected light was detected by an InGaAs photodetector. The dc output of the InGaAs photodiode was kept constant by a servomechanism of variable neutral density filter. A SIGNAL RECOVERY model 7265 dual phase DSP lock-in amplifier was used to extract the detected signals. The entire data acquisition procedure was performed under computer control. Multiple scans over a given photon energy range were programmed until a desired signal-to-noise level has been obtained. For temperature-dependent measurement, a closed-cycle cryogenic refrigerator equipped with a digital thermometer controller with temperature stability better than 0.5 K was used.

3. Results and Discussion

Figures 1(a) and 1(b) show the experimental PR spectra (dotted lines) of Ge/Si$_{0.16}$Ge$_{0.84}$ MQW structure at 10 and 300 K, respectively. In order to identify the strain type of Ge-on-Si VS, the PR spectra of Ge bulk and MQW removed sample are also included. The experimental PR spectra were fitted with the first-derivative Lorentzian line shape (FDLL) function. The solid curves are the least-squares fits to FDLL function of the form [20–22]

$$\frac{\Delta R}{R} = \mathrm{Re} \sum_{j=1} A_j e^{i\Phi_j} \left(E - E_j + i\Gamma_j\right)^{-n}, \quad (1)$$

where A_j and Φ_j are the amplitude and phase of the line shape, E_j and Γ_j are the energy and broadening parameter of the transitions, and the value of n depends on the origin of the transitions. For the derivative functional form,

$n = 2$ is appropriate for the bound states such as excitons. The obtained transition energies from (1) with $n = 2$ were indicated by arrows.

In Figure 1, we compare the PR spectra of Ge bulk and MQW removed sample. As shown in Figures 1(a) and 1(b), the near direct band edge transition of Ge bulk is located at 0.892 ± 0.005 and 0.804 ± 0.005 eV at 10 and 300 K, respectively. In Figure 1(a), we can clearly observe double transitions from MQW removed sample and full Ge/$Si_{0.16}Ge_{0.84}$ MQW structure above ~0.9 eV. By comparing the spectra with Ge bulk, the two distinct peaks observed in MQW removed sample and full Ge/$Si_{0.16}Ge_{0.84}$ MQW structure were blue shifted. The two peaks can be attributed to transition from the heavy-hole state to the conduction band state at Γ point (hh-Γ) and that from the light-hole state to the conduction band state at Γ point (lh-Γ), indicating the compressive built-in strain in Ge-on-Si VS. Besides the hh-Γ and lh-Γ near band edge transitions due to the strain-splitted valence bands of Ge VS, PR spectra reveal three *mn*H(L) quantum-confined interband transitions from full MQW structure, where *mn*H(L) denotes a transition between the *m*th conduction band state at the Γ point and the *n*th heavy (H)- or light (L)-hole valence band state. The determined quantum-confined interband transition energies for 11H, 11L, and 22H at 300 K are 0.868 ± 0.005, 0.900 ± 0.005, and 0.976 ± 0.005 eV, respectively.

Figure 2 depicts the schematic band line-up and various quantum-confined states at the conduction and valence bands in Ge/$Si_{0.16}Ge_{0.84}$ MQW structure. We show the conduction band edge and the valence band edges (heavy-hole and light-hole bands) at the Γ point. The corresponding band offsets of the conduction, heavy-hole valence, and light-hole valence bands are denoted by ΔE_c, $\Delta E_{v,\mathrm{hh}}$, and $\Delta E_{v,\mathrm{lh}}$, respectively. In order to specify the obtained *mn*H(L) features, we have solved the one dimensional Schrödinger equation for finite quantum wells based on the envelope function approximation [23] including the effects of strain. The relevant parameters such as effective masses of electron, heavy-hole and light-hole, the lattice constant, hydrostatic *(a)* and shear *(b)* deformation potentials, and the elastic stiffness constants C_{11} and C_{12} of the ternary material are listed in Table 1 with their corresponding references. The parameters of the binary material were obtained by linear interpolation of values of the end-point elements Ge and Si. A reasonable agreement is found between experiments and theoretical calculations. In our calculations, the conduction band-offset ratio is defined as $Q_c = \Delta E_c/(\Delta E_c + \Delta E_v)$. The conduction band-offset ratio $Q_c = \Delta E_c/(\Delta E_c + \Delta E_v)$ varied in the range of 0.63–0.68, as suggested by previous studies [16, 24–26]. In this study, we found that the best agreement between experimental results and theoretical calculations can be achieved by taking $Q_c = 0.63$.

We have also studied the temperature dependence of the near band edge transitions of Ge-VS and various quantum-confined interband transitions in the temperature range of 10–300 K. For comparison, the temperature-dependent PR measurements in the vicinity of band edge of Ge bulk were also carried out. Figure 3(a) shows the near band edge PR spectra of bulk Ge. Figure 3(b) shows the hh-Γ and lh-Γ

Table 1: Parameters of band gap energy, strain related constants, and effective mass for the Ge/SiGe material system.

Parameter	Symbol (unit)	Si	Ge	Reference
Lattice constant	a_0 (Å)	5.431	5.657	[30]
Band gap energy	E_g (eV)	4.06	0.802	[31, 32]
Hydrostatic deformation potential	a (eV)	−0.48	−8.97	[33, 34]
Shear deformation potential	b (eV)	−2.3	−1.88	[33, 34]
Elastic stiffness constant	C_{11} (10^{11} dyn/cm^2)	16.57	12.4	[35, 36]
Elastic stiffness constant	C_{12} (10^{11} dyn/cm^2)	6.39	4.13	[35, 36]
Electron effective mass	m_e/m_0	0.188	0.045	[37, 38]
Heavy-hole effective mass	m_{hh}/m_0	0.528	0.284	[37, 39]
Light-hole effective mass	m_{lh}/m_0	0.157	0.044	[37, 39]

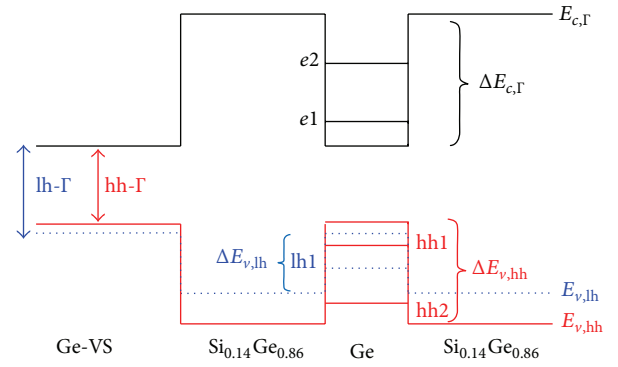


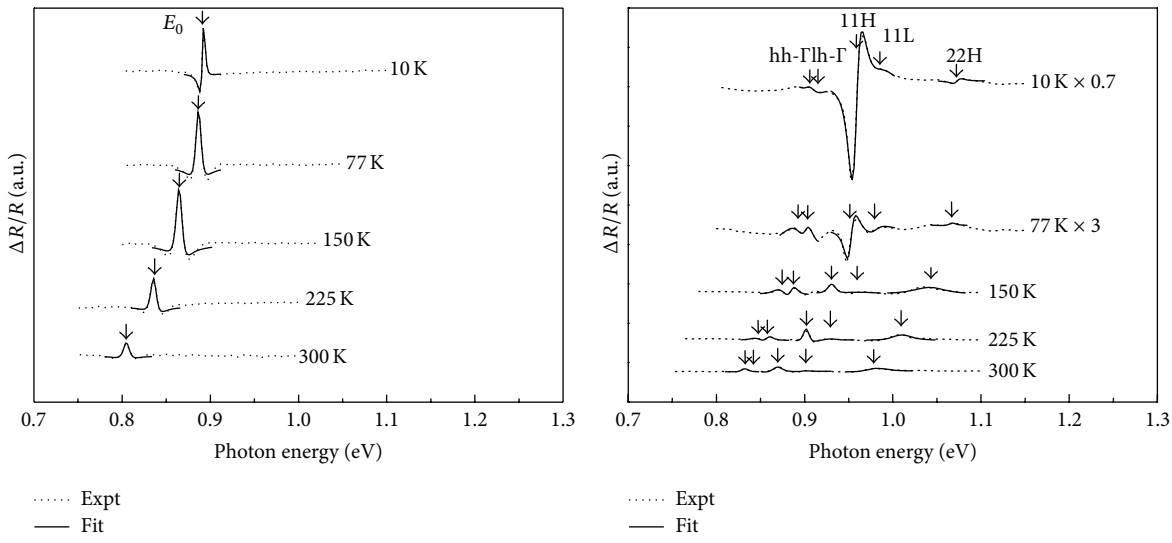
Figure 2: The schematic band diagram of Ge/$Si_{0.16}Ge_{0.84}$ MQW structure for 11/26 nm well/barrier width. The conduction and valence band edges and electron, and heavy- and light-hole quantum-confined states are shown.

related PR spectra caused by strain-induced valence band splitting of Ge VS and three quantum-confined interband transitions from Ge/SiGe MQW structure. The solid curves show the fitted spectra obtained from (1) with $n = 2$. The corresponding transition energies are indicated by the arrows. As expected, the near band edge and quantum-confined interband transition peaks of three observed features show a red shift with an increase of temperature.

We further study the temperature-dependent PR spectra of various quantum-confined interband transitions in the temperature of 10–300 K. Figure 4 plots the temperature dependence of Ge bulk and $E_{mn\mathrm{H(L)}}(\mathrm{T})$ transition energies determined from PR spectra. The dashed lines represent the least-squares fits to the Varshni semiempirical expression [27]

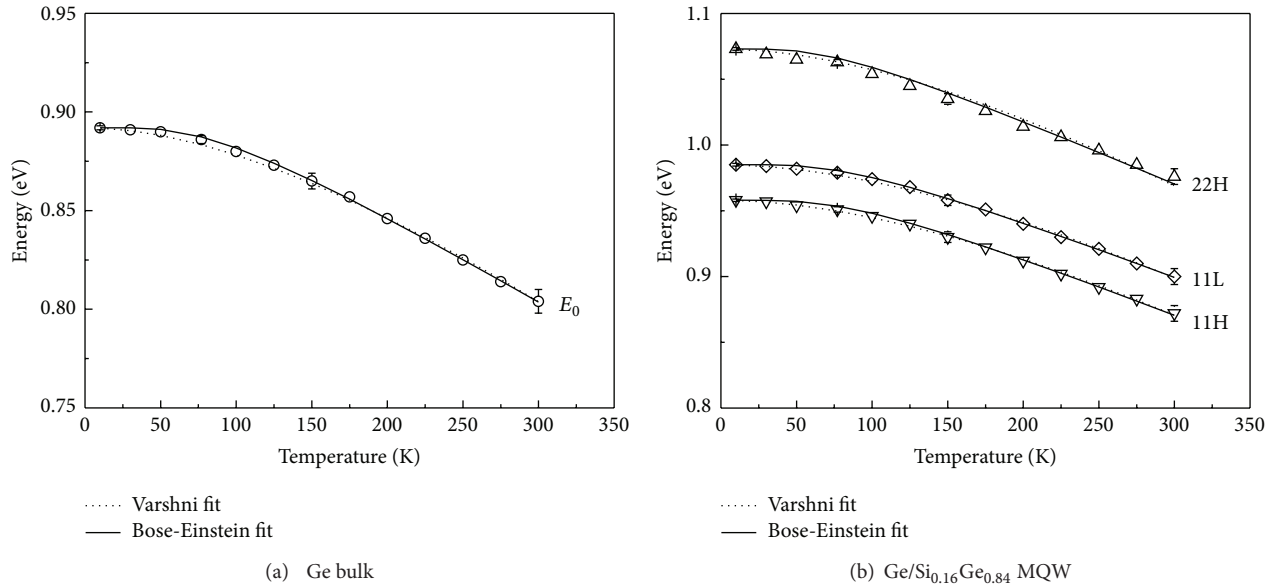
$$E_i(\mathrm{T}) = E_i(0) - \frac{\alpha_i \mathrm{T}^2}{\beta_i + \mathrm{T}}, \quad (2)$$

where $E_i(0)$ is the quantum-confined interband transition energy for *mn*H(L) at 0 K. The constant α_i is related to the electron (exciton) phonon interaction strength and β_i



(a) Ge bulk (b) $Ge/Si_{0.16}Ge_{0.84}$ MQW

FIGURE 3: Temperature-dependent PR spectra for (a) Ge bulk and (b) $Ge/Si_{0.16}Ge_{0.84}$ MQW structure at several temperatures between 10 and 300 K. The dashed curves are the experimental curves and the solid curves are the least-squares fit to the first-derivative Lorentzian line shape.



(a) Ge bulk (b) $Ge/Si_{0.16}Ge_{0.84}$ MQW

FIGURE 4: The temperature variations of various transition energies for (a) Ge bulk and (b) $Ge/Si_{0.16}Ge_{0.84}$ MQW structure with representative error bars. The dashed curves are least-squares fits to the Varshni semiempirical expression. Solid curves are the least-squares fits to the Bose-Einstein expression.

is closely related to the Debye temperature. The obtained values of $E_i(0)$, α_i, and β_i are listed in Table 2.

We have also fitted the experimental transition energies to the Bose-Einstein expression (solid lines in Figure 4) [28]

$$E_i(\mathrm{T}) = E_i(0) - \frac{2a_{Bi}}{\left[\exp\left(\Theta_{Bi}/\mathrm{T}\right) - 1\right]}, \quad (3)$$

where $E_i(0)$ is the transition energy for mnH(L) at 0 K, a_{Bi} represents the strength of the electron (exciton) phonon interaction, and Θ_{Bi} corresponds to the average phonon temperature. The values of various fit-determined parameters are also listed in Table 2. For comparison, the literature values for Ge/SiGe MQW [17, 29] and those of Ge bulk [29] are also included in Table 2.

The parameter α_i in (2) is related to a_B and Θ_B in (3) in the high-temperature limit of both expressions. This yields $\alpha = 2a_B/\Theta_B$. Values in Table 2 show that this relation is satisfied approximately. From (3), it is straightforward to show that high-temperature limit of the slope of $E_{mn\mathrm{H(L)}}(\mathrm{T})$ versus T curve approaches a value of $-2a_B/\Theta_B$. The calculated values of $-2a_B/\Theta_B$ for $E_{mn\mathrm{H(L)}}$ quantum-confined interband transition

Table 2: Values of the Varshni- and Bose-Einstein-type fitting parameters, which describe the temperature dependence of the *mn*H(L) transitions of Ge/SiGe MQW. The direct gaps of bulk Ge also included for comparison.

Samples	Feature *mn*H(L)	$E_{mn\mathrm{H(L)}}(0)$ (eV)	α_i ($\times 10^{-4}$ eV/K)	β_i (K)	a_{Bi} (meV)	Θ_{Bi} (K)	$dE_{mn\mathrm{H(L)}}/d\mathrm{T}$ (meV)
$Ge/Si_{0.16}Ge_{0.84}$ MQW[a]	11H	0.958 ± 0.003	7.5 ± 0.8	453 ± 50	61 ± 10	256 ± 30	−0.41
	11L	0.985 ± 0.003	7.5 ± 0.8	485 ± 50	57 ± 10	254 ± 30	−0.38
	22H	1.073 ± 0.003	8.0 ± 0.8	445 ± 50	63 ± 10	250 ± 30	−0.43
$Ge/Si_{0.15}Ge_{0.85}$ MQW[b]	11H	0.968 ± 0.003	7.4 ± 0.8	430 ± 100	59 ± 10	250 ± 30	−0.45
	11L	1.011 ± 0.003	7.2 ± 0.8	400 ± 100	56 ± 10	245 ± 30	−0.44
	22H	1.037 ± 0.003	6.9 ± 0.8	430 ± 100	55 ± 10	250 ± 30	−0.41
$(Si_4Ge_6)_5Ge_{78}$ MQW[c]	11H	0.957 ± 0.003	7.2 ± 1.5	420 ± 150	65 ± 10	290 ± 46	−0.43
	11L	0.984 ± 0.003	6.8 ± 1.5	370 ± 150	60 ± 10	255 ± 46	−0.41
Ge bulk[a]	E_0	0.892 ± 0.005	6.7 ± 0.8	386 ± 50	57 ± 10	251 ± 30	−0.41
Ge bulk[c]	E_0	0.885 ± 0.002	6.5 ± 0.7	410 ± 100	66 ± 12	298 ± 35	−0.38

[a]This work (photoreflectance).
[b]Reference [17] (piezoreflectance).
[c]Reference [29] (piezoreflectance).

energies are −0.48, −0.44, and −0.50 meV/K for 11H, 11L, and 22H, respectively, which agree well with the values of $[dE_{mn\mathrm{H(L)}}/d\mathrm{T}]$ = −0.41, −0.38, and −0.43 meV/K obtained from the linear extrapolation of the high-temperature (150–300 K) PR data. The obtained parameters of the temperature dependence of $E_{mn\mathrm{H(L)}}(\mathrm{T})$ in the present $Ge/Si_{0.16}Ge_{0.84}$ MQW samples are comparable with the previous Ge/SiGe MQW values [17, 29]. In agreement with the same material systems, the values for the parameters that described $E_{mn\mathrm{H(L)}}(\mathrm{T})$ of MQWs in this study are found to be similar to those of the constituent bulk well-material (Ge).

4. Conclusions

We have studied the temperature-dependent PR spectra of $Ge/Si_{0.16}Ge_{0.84}$ MQW structure and Ge bulk in the range of 10–300 K. The strained-induced hh-Γ and lh-Γ near band edge transitions originating from the valence band splitting in Ge-on-Si VS have been observed. Compared to Ge bulk material, the valence band splitting and band edge blue-shift indicate that the Ge-on-Si VS is under compressive strain. The PR spectra also display a number of features originating from quantum-confined interband transitions from the $Ge/Si_{0.16}Ge_{0.84}$ MQW structure. Theoretical calculations based on envelope function approximation were performed to identify the quantum-confined states in $Ge/Si_{0.16}Ge_{0.84}$ MQW structure. Good agreement between experimental results and theoretical calculations can be achieved by taking into account the conduction band offset ratio of Q_c = 0.63. The obtained parameters of the temperature dependence of $E_{mn\mathrm{H(L)}}(\mathrm{T})$ are found to be nearly the same as those of constituent bulk well-material (Ge).

Acknowledgments

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