Optical and structural investigation of SiGe/Si quantum wells

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In this letter we report photoluminescence and structural results obtained on asymmetrically strained $Si_{0.7}Ge_{0.3}/Si$ single and multiple quantum wells epitaxially grown by low pressure chemical vapor deposition. Well-resolved peaks were obtained which can be attributed to quantum well excitons and their transversal optical phonon replica. A good correlation between peak properties and structure results was found. From the photoluminescence peak energies a valence band offset of 0.27 eV and an effective hole mass of 0.25 were estimated.

Photoluminescence (PL) is a powerful method widely used in later years to study the electronic states in quantum wells. For SiGe/Si heterostructures there have been several reports of PL for various samples from unstrained bulk to atomic layer superlattices. For unstrained bulk $Si_{1-x}Ge_x$ alloys Weber and Alonso[1] presented a detailed study of the near-band-gap PL. Sharp lines were detected in unstrained $Si_{1-x}Ge_x$ alloys grown by liquid phase epitaxy.[2] Broad PL peaks were detected on molecular beam epitaxy (MBE) grown single layers.[3,4] Intense PL was reported by Noël *et al.*[4] for MBE-grown single (SQW) and multiple quantum wells (MQW). There are several reports on strained $Si_m Ge_n$ superlattices grown by MBE.[5–7] In particular, it has been predicted that for certain values of m and n and specific strain conditions, direct or quasi-direct band-gap material should be obtained in these superlattices.[8]

In the present study, SiGe/Si SQWs and MQWs were epitaxially grown by low pressure chemical vapor deposition (LPCVD) and characterized by PL, Rutherford backscattering (RBS), and transmission electron microscopy (TEM). We observe several well-defined PL lines at low temperatures, with linewidths of ~7–30 meV depending on quantum well (QW) thickness. The comparison between measured and calculated PL energies allowed us to estimate the valence-band offset (ΔE_V) and the effective mass for holes (m_h^*).

The QW structures were deposited on p-type Si (100) wafers, 2000 Ω cm. The epitaxy was carried out at 700 °C and 0.1 Torr in a LPCVD system[9] using as source gases dichlorosilane and germane. Usual growth rates were for Si 2 nm/min and for $Si_{0.7}Ge_{0.3}$ 1.8 nm/min.[10]

The following layer sequences were chosen: for the MQWs: ~260 nm $Si_{0.93}Ge_{0.07}$ buffer and then the MQWs consisting of $Si_{0.7}Ge_{0.3}$ wells and Si barriers (see Table I) and for SQWs: ~1 μm Si layer, a $Si_{0.7}Ge_{0.3}$ SQW layer, and a $Si_{0.98}Ge_{0.02}$ cap layer (see Table II).

The thickness of the QWs was determined by RBS using 1.4 MeV $^4He^+$ ions, tilting the sample 81° to the He^+ beam and fitting the measured data with calculated ones using the program RUMP.[11] TEM characterization of the SQW and MQW structures was performed with a JEOL 4000FX electron microscope at 400 kV on plan-view and cross-section specimens. The PL was measured at 4.2 K using a Fourier transform spectrometer with a Ge *p-i-n* diode cooled with liquid nitrogen as a detector. The samples were optically excited by Ar^+ laser light with a power density of ~10 W/cm^2.

In Fig. 1 typical PL spectra from $Si_{0.7}Ge_{0.3}/Si$ MQWs of various well thicknesses are presented, together with the PL spectrum of the Si substrate itself. Three main features are observed in the PL spectra of the MQWs. We group them into lines labeled from *a* to *d*, lines *D*, and lines from the substrate. Visible in the pure-substrate PL spectrum is a complex of exciton lines. This consists of free exciton lines (FE) with phonon participation (TO, LO, TA, TO $+O_\Gamma$) and bound excitons without phonon and its phonon replica.[12] The broad feature labeled EHD is due to the electron-hole-droplet. All these substrate lines were observed, with one exception, in the MQW spectra, too, but reduced in intensity. The exception is the EHD line, which is absent in all MQWs.

First, we will discuss lines *a* to *d* (see also Table I). Line *d* is well resolved in the 1 nm MQW, in the 1.2 nm sample it lies in the region of substrate lines, in the 1.5 and 2 nm samples it is again well defined. The line *c* overlaps the substrate lines in the 1 nm sample, but for thicker wells it is again well separated from the substrate lines. The dominant characteristic of all four lines *a* to *d* is their shift to lower energy as the well thickness increases, which undoubtedly can be correlated with transitions of electrons from the condition band to QW-confined holes. The linewidth of lines *a* to *d* is for MQWs up to 1.5 nm relatively small (7–10 meV), while broadening occurs for the 2 nm MQW. Another interesting characteristic is that lines *a* and *c* seem to be correlated. Their energy difference is ~57

TABLE I. Data for MQW samples: thickness d (in nm) and PL peaks. For all MQWs: buffer $x=0.07$, $d=260$ nm; QW: $x=0.3$; n is the number of periods.

MQW			PL lines (meV)					
d_{SiGe}	d_{Si}	n	a	b	c	d	$d–b$	$c–a$
1.0	12	10	1031	1051	1089	1109	58	58
1.0	12	20	1031	1050	1089	1109	58	58
1.2	14	20	1021	1034	1078	1093	59	57
1.5	13	20	1008	1017	1064	1075	58	56
2.0	14	20		984	1026	1041	57	

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TABLE II. Data for SQW samples: thickness d and energies of PL lines; cap layer: $x=0.02$; SQW: $x=0.3$.

Cap layer d/nm	SQW d/nm	PL lines/meV a	b	c	d	d–b
360	2.2		977	1018	1034	57
500	2.6		912		963	51
580	2.7		894		947	53
330	3.5		888		938	50
17	5.0		865		920	55
13	5.8		959		914	55

meV, while the same is valid for the line pair b and d having an energy difference of ~ 58 meV.

The lines D_1 and D_2 do not shift when the well thicknesses increase, but they become more intense for thicker wells. Their energetic position coincides with the dislocation lines D_1 (0.812 eV) and D_2 (0.875 eV) identified in deformed silicon[13] and were also observed in relaxed SiGe.[4,7]

Figure 2(a) presents a MQW structure with wells of 1.5 nm thickness in a cross-section TEM micrograph showing a high degree of perfection characterized by layers of homogeneous thickness and abrupt and planar interfaces. This demonstrates, that this MQW structure is fully strained. A network of misfit dislocations has been identified at the buffer-substrate interface, visible as localized strained regions, which are undoubtedly related to the D_1 and D_2 lines in the PL spectrum of this sample. Figure 2(b) shows a cross-section TEM micrograph of a 2 nm MQW structure displaying regions of high structural perfection and regions within the individual wells with a continuously changing well thickness and/or composition, resulting in increasing bulging of the multilayers in growth direction. Misfit dislocations are present only at the buffer-

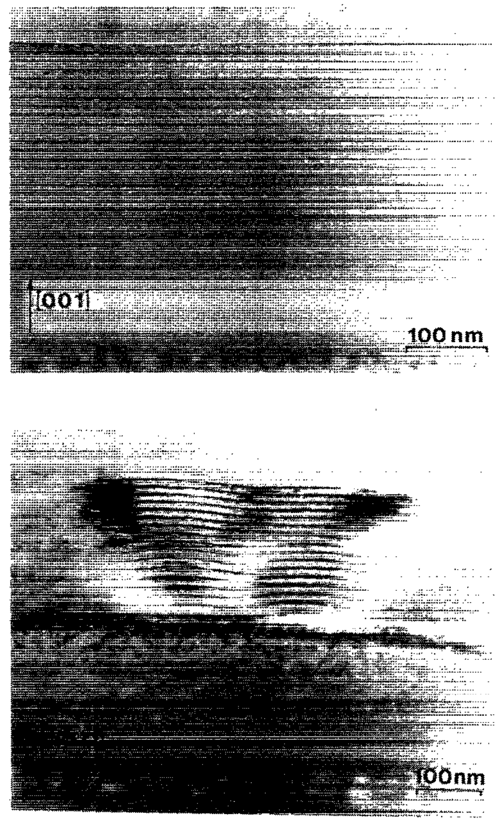

FIG. 2. Cross-section TEM micrograph of 20-period MQW structures grown on $Si_{0.93}Ge_{0.07}$ buffers; bright field images were taken with electron beam parallel to interfaces near a ⟨110⟩ projection. The corresponding PL are shown in Fig. 1. Nominal well width: (a) 1.5 nm and (b) 2 nm.

substrate interface, but not at all at the well interfaces and no threading dislocations were observed. The formation of such regions (lateral extension $\sim$100–500 nm) was observed for all samples with nominal thickness of the SiGe wells >2 nm. It also occurred in SQWs, if this layer thickness is exceeded.

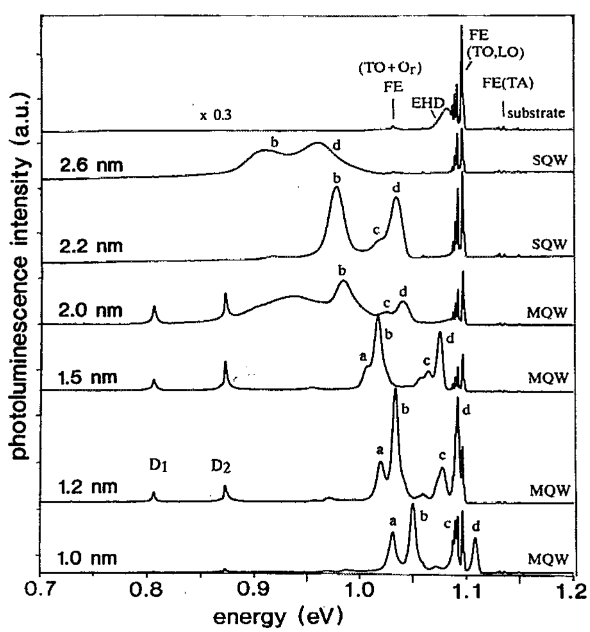

FIG. 1. PL spectra of $Si_{0.7}Ge_{0.3}$/Si MQW and SQW structures with different well thicknesses and of the substrate alone, measured at $T\sim 4.2$ K.

The SQWs investigated have a nominal well thickness of 2.2 to 6 nm (see Table II). In Fig. 1 PL spectra of two SQW structures are shown. Similar to the MQWs, the QW-related lines b to d of the SQW samples shift to lower energy as the well becomes thicker, and for wells >2.5 nm only lines d and b are detected, with an energy difference of ~ 55 meV. No dislocation lines were detected for all SQWs investigated (see Table II). Similar to the MQWs, inhomogeneous regions are also observed by TEM for all SQWs investigated, but no misfit dislocations at the interfaces and no threading dislocations are detected which explains the absence of the D_1 and D_2 lines in the PL spectra of the SQWs. We can conclude, that for the SQW and MQW structures based on asymmetrically strained $Si_{0.7}Ge_{0.3}$/Si the inhomogeneities in the SiGe layers were obviously the cause for the broadening of the PL lines b and d and the disappearance of lines a and c.

We start the discussion with the PL lines a and b. Tables I and II show, that these lines lie 50–58 meV below the c and d lines. In bulk $Si_{1-x}Ge_x$ alloys Weber and Alonso[1] identified the $TO_{Si\text{-}Si}$ phonon with 58 meV and the

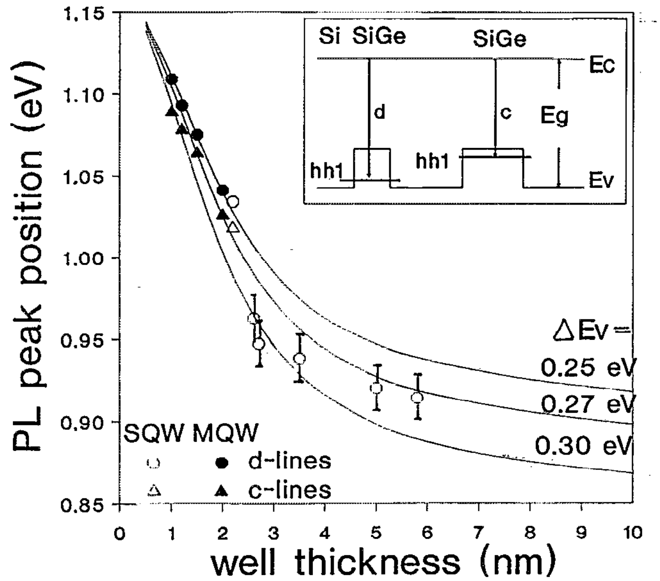

FIG. 3. Calculated and experimental PL peaks as a function of the well thickness. Only no-phonon QW exciton lines *c* and *d* are represented. (a) ●, ▲ MQW, (b) ○,△ SQW.

$TO_{Si\text{-}Ge}$ with 49 meV. This allows us to interpret lines *a* and *b* as TO replicas of the PL lines *c* and *d*, respectively. The *c* and *d* lines we assign to no-phonon transitions due to QW excitons, splitted into a doublet. Doublet splitting in the photoluminescence spectra of III-V heterostructures was explained as being due to 1 monolayer thickness variation if the lateral extension of the thickness fluctuations is greater than the Bohr radius of the confined excitons.[14] In our case, the QW exciton lines *c* and *d* lie ~20 meV apart, which is equivalent to ~2 monolayers thickness variation. This was observed for well thicknesses <2 nm.

In order to analyze the no-phonon QW-exciton lines more quantitatively, we calculate the quantized state energies E_i in the QW using different values for m_h^* in the well and the barrier. No dependence on strain of m_h^* was taken into account. The energetic position of the PL lines is equal to $E_g-\Delta E_V+E_i$ and is represented in Fig. 3 as a function of the well thickness for $i=1$. Here E_g is the gap for cubic Si. Also represented are the QW-exciton lines *c* and *d*. A reasonable fit was obtained with $m_h^*=0.25$ m and $\Delta E_V=0.27$ eV. The disappearance of splitting for wells >2.5 nm and broadening of the QW-exciton line *d* is due to an increase of thickness fluctuations, which is in agreement with the TEM results.

In conclusion, the photoluminescence of asymmetrically strained $Si_{0.7}Ge_{0.3}/Si$ MQW and SQW structures is due to QW excitons and their TO replicas indicating the indirect character of this system. It was possible to estimate a valence band offset of 0.27 eV and an effective hole mass of 0.25 m. Splitting of the no-phonon QW-exciton lines is very probably due to thickness fluctuations. In addition, we found that the PL dislocation lines D_1 and D_2 are well correlated with misfit dislocations at the buffer substrate interface.

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