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# Photoluminescence of a tensilely strained silicon quantum well on a relaxed SiGe buffer layer

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We have investigated the photoluminescence of tensilely strained silicon layers grown on relaxed SiGe buffer layers. At low excitation densities, the photoluminescence is dominated by the radiative recombinations associated with the dislocations in the buffer layer and the band-edge luminescence of the relaxed SiGe layers. We show that the photoluminescence of a strained silicon quantum well capped by a relaxed SiGe layer can be observed at high excitation densities. The resonance energy of this photoluminescence, observed around 960 meV for the phonon-assisted transition, is in satisfying agreement with the calculated value of the bandgap of the type II strained heterostructure. © *2004 American Institute of Physics*. [DOI: 10.1063/1.1766073]

Strained silicon on relaxed SiGe layers has been extensively studied in recent years for its application in microelectronic devices. The enhanced carrier mobility in tensilely strained Si channel layers allows the development of high performance metal-oxide-semiconductor field-effect transistors or *n*-type modulation doped field-effect transistors.[1] The combination of tensilely-strained silicon with SiGe on insulator offers new opportunities to develop high frequency devices with low noise performance.[2] The enhanced performances with tensilely strained Si layers are associated with the better electron confinement at the heterointerface between Si and SiGe and to the splitting of the degeneracy of the $\Delta$ conduction valleys.[3] The measured values of ohmic mobilities can be as high as $5\times10^5$ cm$^2$/V s at low temperature for strained Si on SiGe and depend on the interface roughness and on the material quality.[4]

It is well known that photoluminescence (PL) is a sound tool to investigate the material properties of silicon-based heterostructures.[5] The dislocations associated with SiGe virtual substrates have been systematically investigated by optical spectroscopy.[6] Band-edge recombination of bound and free excitons in relaxed SiGe layers have been clearly identified.[7] While the electrical properties of tensilely-strained silicon layers have been thoroughly investigated, only few reports have evidenced the band-edge luminescence of strained silicon in a SiGe relaxed matrix.[8,9]

In this work, we report on the band-edge luminescence of a tensilely strained silicon quantum well embedded in a relaxed SiGe matrix. At low excitation densities, besides the dislocations associated with the virtual substrate, we observe the band-edge luminescence of the relaxed SiGe layer. We show that at high excitation densities, new recombination lines appear that are associated with the strained Si quantum well.

The investigated samples were grown by reduced pressure chemical vapor deposition on 8-in. (001) oriented Si substrates.[10] The growth pressure was 20 Torr. The growth temperature was 750 °C. Dichlorosilance and germane diluted at 2% in $H_2$ were used as gaseous precursors for silicon and germanium. Several types of structures were grown: Thick, nearly fully relaxed constant composition (20%–31%) SiGe layers were grown on linearly graded SiGe layers i.e., SiGe virtual substrates), with (i) or without (ii) uncapped, tensilely strained silicon layers sitting on top. For some of the samples, modulation doped tensilely strained Si quantum wells (iii) were instead embedded in the relaxed SiGe layers of our virtual substrates. In case (iii), two different Ge contents were investigated: 20% and 31%. The thickness of the Si quantum well was 12 nm for 20% of Ge and 8 nm for 31% of Ge. In the following, we have chosen to highlight the results obtained with a structure that shows evidence of tensilely strained silicon PL. The structure consists of a graded SiGe buffer layer with a 8% Ge/$\mu$m grading, a relaxed $Si_{0.8}Ge_{0.2}$ layer more than 1 $\mu$m thick, a strained silicon channel layer 12 nm thick, and a relaxed SiGe cap layer 62 nm thick. The SiGe cap layer contains a n-type modulation phosphorous doping 30 nm thick with a carrier concentration of $3\times10^{18}$ cm$^{-3}$. The modulation doping is separated from the Si quantum well by a 20-nm-thick intrinsic SiGe layer. The 12-nm-thick SiGe layer on top of the modulation doping is nominally undoped. The whole structure is capped by a 2-nm-thick silicon layer. The PL was excited with an $Ar^+$ laser.

Figure 1 shows a low temperature PL spectrum in linear scale obtained under weak excitation conditions ($\sim$0.4 W cm$^{-2}$). The relaxed SiGe layer composition is 20%. The PL is dominated at low energy by dislocation-related recombination lines. The lines resonant at 804, 854, and 924 meV correspond to the D1, D2, and D4 recombinations, respectively. These energies are consistent with the reported values of the dislocation-related D lines for a germanium content around 22%–23%.[6] At higher energy, we observe the bound exciton recombination in the relaxed SiGe layer, with the no-phonon recombination at 1064 meV and the recombination assisted by a TO phonon at 1006 meV. These values of near-band-edge PL energy for a 20% relaxed SiGe layer are also consistent with previously reported data in the literature.[7] The small features observed between these two

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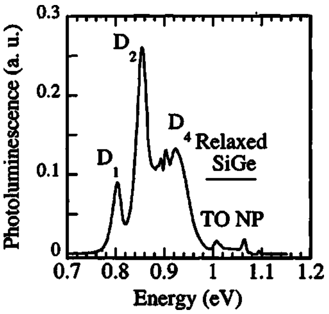

FIG. 1. 3 K PL spectrum of the heterostructure containing a strained silicon layer on a relaxed $Si_{0.8}Ge_{0.2}$ buffer layer. The power excitation density is 0.4 W $cm^{-2}$.

recombination lines at 1028 and 1046 meV correspond to the Ge-Ge TO phonons and to the TA phonon replicas, respectively. A weak recombination is also observed at 1094 meV. It corresponds to the phonon-assisted replica TO of the bound exciton recombination in the Si substrate.

Figure 2 shows the low temperature PL in log scale as a function of the power excitation density. The luminescence of the dislocation lines grows sublinearly as a function of the excitation density. Above 10 W $cm^{-2}$, a small peak is observed around 960 meV. The amplitude of this peak increases superlinearly, with a square dependence of the amplitude measured after background substraction as a function of the power excitation. This resonance comes with an additional peak observed at 1018 meV for a 20 W $cm^{-2}$ excitation, that is, 58 meV above. This resonance at 1018 meV follows the same power dependence as the 960 meV line. Both recombination lines shift to higher energy as the power excitation density is increased, with a ~9 meV blueshift when going from 12 up to 32 W $cm^{-2}$. An increase of the broadening of the lines is also observed. Meanwhile, we observe that the band-edge recombination in the SiGe relaxed layer vanishes at high excitation densities. The decrease of the amplitude of the no-phonon recombination in the relaxed SiGe layer (Fig. 2) at high excitation densities is attributed to the carrier diffusion and their redistribution in the heterostructure. As explained later, we assign the recombination lines around 960 and 1018 meV to the phonon-assisted and to the no-phonon recombinations in the tensilely strained Si channel respectively. These recombinations were not observed in samples without the Si quantum well, (i.e., relaxed SiGe layers on a graded buffer layer), and in samples with an uncapped Si quantum well deposited on top of a relaxed SiGe layer. In the case of the modulation-doped strained Si heterostructure embedded in a layer with a nominal 31% Ge content, we did observe the band-edge recombination of the relaxed $Si_{0.69}Ge_{0.31}$ layer at low excitation with a no-phonon luminescence peaked at 1032 meV. At high excitation densities, we did not observe additional recombination lines in the PL spectra, thus ruling out the modulation doping as the origin of the 960 and 1018 meV lines. The energy difference between these two transitions corresponds to the TO phonon energy in silicon. We also rule out that these two recombinations might be associated with the D5 and D6 straight dislocations and stacking faults that can be observed under specific stress conditions.[11] First, these transitions are resonant in silicon at 953 and 1012 meV; that is, at a smaller energy. Second, these emission features usually come with an additional emission (D′5) around 900 meV that is not observed in the present case. The superlinear emission as a function of the power excitation density suggests that the 960 and 1018 meV lines are not associated with defect recombination.

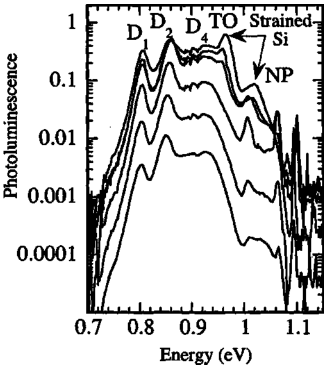

FIG. 2. 5 K PL as a function of the power excitation density (log scale). From bottom to top: 0.02, 0.2, 2, 12, 20, 32 W $cm^{-2}$.

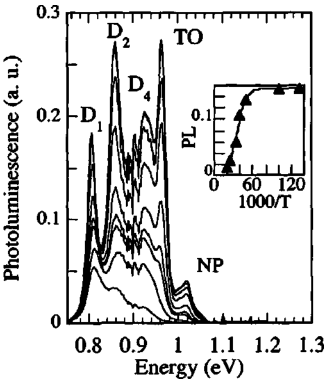

FIG. 3. PL as a function of the temperature. From top to bottom: 7.5, 10, 20, 25, 30, 40, 50, 70, 90 K. The power excitation density is 20 W $cm^{-2}$. The inset shows the fit of the PL amplitude of the TO line of the strained Si layer around 960 meV as a function of the temperature.

Figure 3 shows the temperature dependence of the PL measured under high excitation conditions. The strained silicon recombination lines vanish above 50 K. The temperature dependence of the PL amplitude $I(T)$ was fitted according to $I(T)=I_0(1+g\,T^{3/2}[\exp(-E_a/k_BT)]^{-1}$, where $I_0$ is the amplitude at 0 K, $E_a$ the activation energy, $k_B$ the Boltzmann constant, $T$ the temperature, and $g$ a fitting parameter.[7] An activation energy $E_a$ of 9 meV was deduced for both the no-phonon and the phonon-assisted recombinations. This small activation energy is associated with the thermionic emission of holes trapped at the heterointerface between the strained Si channel and the relaxed SiGe layer.

The band structure of tensilely strained silicon on a relaxed SiGe matrix has been calculated by several authors.[12–14] The strain splits the degeneracy of the conduction band between the $\Delta_2$ valley along the growth axis and the in-plane $\Delta_4$ valleys. The splitting is around 120 meV for a 20% Ge content buffer. The conduction band discontinuity between the $\Delta_2$ valley in silicon and the $\Delta_4$ valleys in SiGe is around 6 meV/% Ge. One thus expects a 120 meV band discontinuity in the conduction band between the strained Si channel and the SiGe 20% relaxed layer. The strain also splits the degeneracy between the light-hole and heavy-hole bands at the Brillouin zone center, the light-hole band shifted above the heavy-hole band. The band gap energy at low tem-

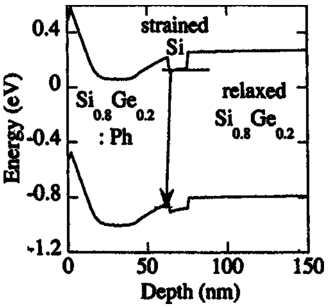

FIG. 4. Calculated energy band diagram of the investigated heterostructure. The recombination path between electrons in the Si channel layer and holes trapped at the heterointerface is indicated by an arrow.

perature of a strained Si layer on a relaxed $Si_{0.8}Ge_{0.2}$ layer was calculated to be at 1016 meV using a 20 **k.p** formalism.[15] Tensilely strained Si on a relaxed SiGe layer corresponds to a type II band alignment, with a valence band offset around 75 meV. Figure 4 shows the calculated band diagram of the heterostructure. The band bending was calculated by solving the Poisson equation. A value of 0.91 $m_0$, where $m_0$ is the free-electron mass, was considered for the longitudinal effective mass of the electrons in the Si channel.[14] In the valence band, a value of 0.27 $m_0$ (0.18 $m_0$) was deduced from the Luttinger parameters for the effective mass of the heavy (light) holes along the growth axis in the relaxed SiGe layer.[16] The effective mass in strained silicon was 0.17 $m_0$ and 0.3 $m_0$ for light and heavy holes, respectively. The valence band offset between relaxed SiGe and strained Si was taken as 75 and 184 meV for the light-hole and heavy-hole bands, respectively. In the calculation, the Fermi level was considered pinned at midgap at the surface. The confinement energy of the electrons in the Si well and of the holes in the triangular well at the SiGe/Si heterointerface depends obviously on the band bending. We have estimated a confinement energy for the electrons of ~15 meV and a confinement energy ~35 meV for the heavy holes. At low temperature, the spatially indirect recombination between the electrons in the Si channel and the holes at the heterointerface between Si and SiGe is thus expected to occur around 990 meV.

We attribute the recombination lines at 1018 and 960 meV to the spatially indirect type II recombination, as indicated in Fig. 4, for the following reasons. As discussed earlier, the energy of the recombination is close to the calculated value. We note that the calculated value depends on the strained silicon bandgap and on the conduction band offset, which were taken as input parameters, as well as on the effective band bending, which depends additionally on the photoinduced carrier density. These features can explain the discrepancy between the calculated value of the recombination and the measured value. The 9 meV activation energy deduced from the temperature-dependent measurements indicates that the hole confinement energy is probably underestimated; that is, the hole confined states are probably closer to the strained silicon valence band edge and the PL should occur at higher energy. The line at 1018 meV corresponds to the no-phonon recombination, while the line resonant at 960 meV with a much larger amplitude corresponds to the phonon-assisted recombination. We rule out a direct type I recombination (electrons and holes) in the Si layer because of the strong band bending. A type II recombination depends on the spatial overlap between the electron and the hole wave functions. This overlap will increase as the band bending is increased at high excitation densities because of the electrostatic interaction between spatially separated electron and holes. One thus expects an enhancement of the recombination at high excitation as it is experimentally observed. Furthermore, we observe a blueshift of the recombination as a function of the excitation density. A similar buleshift has already been reported for type II recombination, either with a quantum confinement for the holes[17] or a quantum confinement for the electrons.[18] We note that in Ref. 9, a redshift of the spatially indirect recombination in the strained Si layer was mentioned as the power excitation increases. The amount of the redshift was, however, dependent on the crystal quality, as evidenced by rapid thermal annealing experiments. The experimentally observed blueshift results from the band bending but also from the band filling, as we do observe an increased linewidth of the recombination as the excitation increases. The high excitation density leads to the formation of an electron hole plasma.[19] We note that the band bending is important in those structures as a result of the long recombination times associated with an indirect transition both in k-space and in real space.

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