Detection of Magnetic Resonance on Photoluminescence from a $Si/Si_{1-x}Ge_x$ Strained-Layer Superlattice

E. Glaser, J. M. Trombetta, T. A. Kennedy, S. M. Prokes, and O. J. Glembocki
Naval Research Laboratory, Washington, D.C. 20375

K. L. Wang and C. H. Chern
Device Research Laboratory, Electrical Engineering Department, University of California, Los Angeles, California, 90024

(Received 11 May 1990)

Optically detected magnetic resonance has been employed for the first time on photoluminescence from a $Si/Si_{1-x}Ge_x$ strained-layer superlattice. Emission bands occur at 0.87 and 0.8 eV. One of the resonances is anisotropic with $g_{\parallel}=4.46\pm0.05$ and $g_{\perp}<0.4$ and is assigned to holes of the $J_z=\pm\frac{3}{2}$ valence band in the SiGe layers. This result demonstrates that at least part of the emission must originate from the superlattice region of these structures.

PACS numbers: 78.65.Gb, 73.20.Dx, 76.70.Hb

There has been much interest recently in the study of layered semiconductor structures composed of materials which have significantly different lattice parameters. These so-called strained-layer structures (e.g., GaSb/AlSb, InGaAs/GaAs, etc.) offer new avenues for band-structure engineering and use in integrated optoelectronic systems.[1] In particular, there has been much attention given to the growth of $Si/Si_{1-x}Ge_x$ heterostructures and short-period Si/Ge superlattices (lattice mismatch $\sim4\%$) because of the potential for optoelectronic devices that emit in the near infrared (1.3–1.6 μm) and for the possibility of faster switching times and larger gains in heterojunction bipolar transistors (HBT's).

There exists a fundamental need to determine the conduction- and valence-band offsets and strain splittings that will govern the optical and transport properties of this system. A dramatic lowering of the indirect band gap, relative to that of unstrained bulk SiGe alloys, has been observed via photocurrent spectroscopy in coherently strained $Si/Si_{1-x}Ge_x$ superlattices grown on (001)Si.[2] Also, the E_0 and E_1 optical transitions have been studied by electroreflectance measurements on similar samples.[3] Recently, photoluminescence (PL) has been observed in short-period Si/Ge strained-layer superlattices with total period ≤ 20 Å.[4-6] Most noteworthy, there is support from these experiments for the existence of a quasidirect energy gap due to predicted zone-folding effects.[7] Overall, little is known about the character of the emission in these structures.

The technique of optically detected magnetic resonance (QDMR) has been employed for the first time on photoluminescence from a $Si/Si_{1-x}Ge_x$ superlattice. The present studies on a structure with total period of 160 Å provide clear evidence that the highest confined-hole subband in the SiGe layers is derived from the $J_z=\pm\frac{3}{2}$ valence band (VB) due to the combined effects of strain and quantum confinement. The g tensor associated with the Zeeman splitting of the hole states is described by $g_{\parallel}=4.46\pm0.05$ and $g_{\perp}<0.4$, where $\parallel$ refers to the superlattice axis. Also, the results demonstrate directly from the magnetic resonance signature of the hole that the emission does originate from the superlattice region in this structure.

The sample investigated in this work was grown by molecular-beam epitaxy at 530 °C on an (001)-oriented Si substrate. The structure was composed on a 1000-Å-thick Si buffer layer followed by alternating layers of $Si_{0.65}Ge_{0.35}$ (40 Å) and Si (120 Å). The total superlattice thickness was 0.96 μm.

The PL emission was excited with 633-nm radiation from a HeNe laser or 476- and 531-nm lines from a Kr^+ laser. The incident power densities were approximately 0.1–1 W/cm^2. The infrared emission was collected through a SPEX $\frac{1}{4}$-m double-grating spectrometer and detected with a Northcoast liquid-nitrogen–cooled Ge photodiode. The sample was immersed in a helium bath ($\sim$1.6 K) in the tail section of an optical cryostat.

The magnetic resonance was detected synchronously as the change in the total photoluminescence intensity which was coherent with the on-off amplitude modulation ($\sim$200 Hz) of 50 mW of microwave power. The experiments were carried out at both 24 GHz (K band) and at 35 GHz (Q band) in conjunction with a 9-in. electromagnet (maximum field strength $=1.1$ T) and an Oxford Instruments 7-T split-coil superconducting magnet, respectively. Angular studies were performed with the applied magnetic field rotated in the $(1\bar{1}0)$ plane.

The effects of strain and quantum confinement on the conduction- and valence-band structure in $Si/Si_{1-x}Ge_x$ superlattices similar to the sample investigated in this work have been predicted by Pearsall *et al.*[3] A schematic representation of the conduction- and valence-band structure is shown in the inset of Fig. 1. Most of the band-gap discontinuity occurs in the valence band.[8] It is

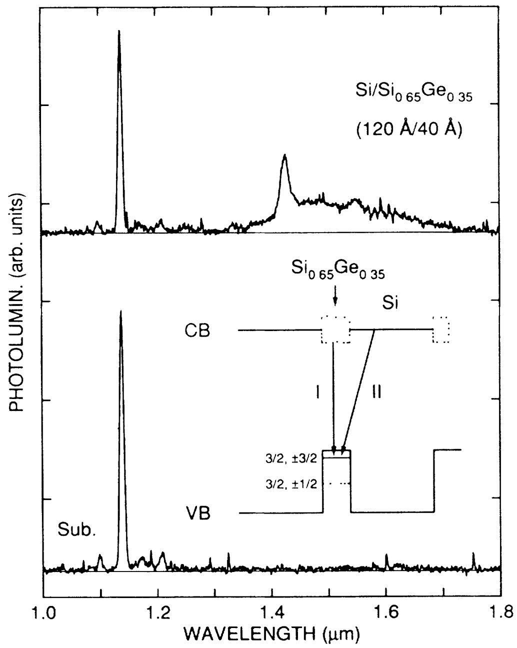

FIG. 1. Photoluminescence spectra of the front (superlattice) and back (substrate) surfaces obtained at 1.6 K with 633-nm excitation. Inset: Schematic representation of energy band structure as described in text. Type-I and -II recombination transitions are both shown due to the uncertainty in the location of the conduction-band (CB) minimum in the superlattice.

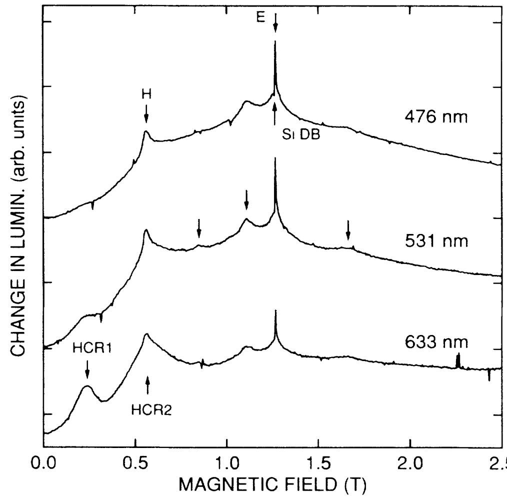

FIG. 2. ODMR spectra obtained at 35 GHz with **B** along the [001] axis for three excitation wavelengths. Peaks are labeled according to the assignments described in the text.

not clear if the electron ground subband level in the present sample is in the Si or SiGe layers after one takes into account the small conduction-band offset. In addition, the $Si_{0.65}Ge_{0.35}$-alloy conduction-band minima are Δ-like (i.e., located along the ⟨100⟩ directions), as in the pure Si layers.[9] The highest hole subband level is located in the SiGe layers. Both the tensile strain in the SiGe layers and the quantum confinement remove the fourfold degeneracy of the $J=\frac{3}{2}$ valence band at Γ leaving two Kramers doublets: $J_z=\pm\frac{3}{2}$ and $\pm\frac{1}{2}$. The combined effects push the $J_z=\pm\frac{3}{2}$ valence band above the $J_z=\pm\frac{1}{2}$ valence band in the SiGe layers (see inset in Fig. 1) by 50 to 100 meV.[3,10]

The PL spectra obtained at 1.6 K with 633-nm radiation incident on the front and back (i.e., substrate) surfaces are shown in Fig. 1. The strong, sharp peak at 1.14 μm (1.09 eV) corresponds to near-band-edge emission from the Si substrate and buffer layer. Two main bands are observed above the base line at lower energies with front-surface excitation only. One of the luminescence bands is found with peak energy at about 1.43 μm (0.87 eV), while a much broader band is observed about 1.5 μm (0.8 eV). The energy of the 0.87-eV band is roughly in agreement with the indirect-energy-gap value obtained from photocurrent spectroscopy measurements[2] on $Si/Si_{1-x}Ge_x$ superlattices with similar parameters and with estimates of the band gap for coherently strained single epitaxial layers of $Si_{0.65}Ge_{0.35}$ on (001)Si.[10]

ODMR spectra obtained at 35 GHz with the applied magnetic field (**B**) along [001] for three values of excitation wavelength (with similar power densities) are shown in Fig. 2. These wavelengths penetrate to different depths of the superlattice. A 1.3-μm-long pass filter was inserted in front of the Ge detector to block the 1.14-μm emission band from the Si substrate and buffer layer in order to study the character of the PL bands at 0.87 and 0.8 eV described above. A variety of resonances were observed. Five of the peaks (HCR1, HCR2, H, E, and Si DB) are labeled according to the assignment of these features discussed below. The identification of three additional (unlabeled) resonances is still under investigation. In addition, the individual resonances obtained at 35 GHz were observed in the 24-GHz spectrometer with the same corresponding g values or effective masses as discussed below.

First, two positive resonances (HCR1 and HCR2) were observed at magnetic fields below 1 T with increasing intensity as the excitation wavelength was varied from 476 to 633 nm. The resonance (HCR1) at ~0.24 T is clearly resolved, while the stronger and broader resonance (HCR2) at higher field underlies a sharper resonance (H) to be discussed below. The increase of the peak intensities with increasing penetration depth of the light, the effective mass values determined from the peak positions of the resonances ($0.18m_0$ and $\sim 0.45m_0$, respectively, where m_0 is the electron mass in free space), and the results of an angular rotation study associate these features with the cyclotron resonance of light and heavy holes in the Si substrate or buffer layer.[11] Since the ODMR with 633-nm excitation shows these bulk resonances, part of the emission that constitutes the 0.87- and 0.8-eV PL bands in Fig. 1 originates from a thick Si region.

Second, a luminescence-quenching resonance labeled Si DB was observed competing with the luminescence-enhancing resonance labeled E. The quenching resonance is much stronger at 24 GHz for reasons not known at the present time. This feature has $g=2.006\pm0.001$ and, thus, is ascribed to Si dangling bonds by comparison with a resonance found in amorphous Si with $g=2.0055\pm0.0005$.[12] The g value associated with dangling bonds in a-$Si_{1-x}Ge_x$ was found previously to be 2.0125 ± 0.0005 (Ref. 13) for samples with the same Ge mole fraction as in the alloy layers of the present sample.

Third, a positive resonance (peak labeled H) was observed with a highly anisotropic g tensor with [001] axial symmetry. The g values (solid circles) of this resonance with the field rotated in the $(1\bar{1}0)$ plane are shown in Fig. 3. The g value was a maximum ($\sim$4.5) with the field along [001] and rapidly approached small values (i.e., $g<0.5$) with the field oriented nearly perpendicular to [001]. For an atomic state with $L=1$, $S=\frac{1}{2}$, and $J=\frac{3}{2}$, the Lande g factor (g^L) is $\frac{4}{3}$.[14] For such a state in axial symmetry, the experimental g values for the $J_z=\pm\frac{3}{2}$ doublet are $g_\parallel=3g^L=4$ and $g_\perp=0$.[15] These are close to the values measured in the Si/SiGe superlattice. The g values for the Kramers doublet with $J_z=\pm\frac{1}{2}$ are $g_\parallel=g^L$ and $g_\perp=2g^L$ (Ref. 14). Thus, the anisotropic resonance (H) is assigned to holes associated with the $J_z=\pm\frac{3}{2}$ valence band in the SiGe layers from the axial symmetry of the g tensor about the [001] axis and the g values obtained with the magnetic field along [001] and nearly perpendicular to [001]. As noted earlier, the combined effects of tensile strain and quantum confinement along the [001] superlattice axis are predicted[3,10] to push the $J_z=\pm\frac{3}{2}$ valence band above the $J_z=\pm\frac{1}{2}$ valence band in the SiGe alloy layers of the present sample. The predicted ordering of the valence-band states in the SiGe layers is explicitly confirmed. The observation of the hole resonance demonstrates that part of the emission does indeed originate from the superlattice region.

The resonance results can be related to Luttinger parameters for the hole states. The spin Hamiltonian that describes the Zeeman splitting of holes in the SiGe layers includes terms both linear and cubic (since $J=\frac{3}{2}$) in the total angular momentum J (Ref. 16),

$$H_h=-2\mu_B\sum(\kappa J_{h,i}+qJ_{h,i}^3)B_i,\quad i=x,y,z\,, \tag{1}$$

where κ and q are the Luttinger parameters and z is both the confinement and tensile strain axis. The magnetic properties of the heavy ($J_{h,z}=\pm\frac{3}{2}$) and light ($J_{h,z}=\pm\frac{1}{2}$) hole bands can be treated separately since the difference in the ground-state subband energies ($\sim$50–100 meV) derived from these bands (including strain effects) are much larger than the Zeeman energies ($\sim$0.1 meV) in this magnetic-resonance experiment. In addition, only the $J_{h,z}=\pm\frac{3}{2}$ states will be occupied at

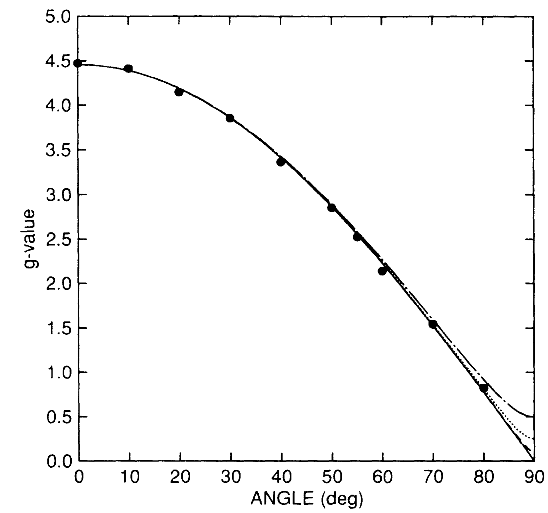

FIG. 3. g value of ODMR feature H as a function of the angle (θ) between **B** and the [001] axis obtained at 24 GHz ($\theta<65°$) and 35 GHz ($\theta>65°$). The curves are fits to the data [see Eq. (3)] with $g'_{h,\parallel}=4.46$ and $g'_{h,\perp}=0$ (solid curve), 0.1 (dashed curve), 0.25 (dotted curve), and 0.5 (dot-dashed curve).

1.6 K. In this case, and because of the reduction in symmetry from cubic to tetragonal, the Zeeman interaction associated with the $J_{h,z}=\pm\frac{3}{2}$ states can be described by a formalism in which the effective spin $S'=\frac{1}{2}$ and the effective spin Hamiltonian can be written as

$$H'_h=\mu_B g'_{h,\parallel}S'_z+\mu_B g'_{h,\perp}(S'_xB_x+S'_yB_y)\,, \tag{2}$$

where $g'_{h,\parallel}$ and $g'_{h,\perp}$ are the g values with the magnetic field applied parallel and perpendicular to the [001] axis, respectively. In Eq. (2), $g'_{h,\parallel}$ is related to both κ and q, while $g'_{h,\perp}$ is related solely to q.[16] Fits have been made (curves in Fig. 3) to the g tensor of the hole resonance for selected values of $g'_{h,\perp}$ with the usual expression for the g values in the case of axial symmetry

$$g'_h=[(g'_{h,\parallel})^2\cos^2\theta+(g'_{h,\perp})^2\sin^2\theta]^{1/2}\,, \tag{3}$$

where θ refers to the angle between B and the [001] symmetry axis. Reasonable fits can be obtained with $g'_{h,\parallel}=4.46\pm0.05$ and $g'_{h,\perp}<0.4$. These g values imply $\kappa+\frac{9}{4}q=0.74\pm0.01$ and $q<0.13$.

Finally, an additional positive resonance (peak labeled E) was observed with $g=1.998\pm0.001$. This value is consistent with measured g values for conduction electrons and shallow donors in bulk Si.[17] This feature is assigned to the spin resonance of electrons located in Si or possibly in the SiGe layers from the g value. The g values of electrons in SiGe alloys are not known at the present time. In addition, the intensity of the feature did not vary significantly with increasing excitation penetration depth, in contrast to the behavior observed for the cyclotron resonance lines. This suggests that the resonance originates from the superlattice region of the sample rather than the Si substrate or buffer layers. The line shape at both 24 and 35 GHz appears to be Lorentzian with a relatively sharp central region and broad wings on the sides of the peak. This is suggestive of donor-acceptor recombination with a distribution of donor-acceptor pair separations. However, there was no evidence of hyperfine interactions (i.e., observation of two or more lines) with narrow field scans in the $g=2$ region as would be anticipated for the magnetic resonance of shallow donors (e.g., P, As, Sb) in Si.

As noted earlier in the discussion of the PL spectra, it is reasonable to ascribe the 0.87-eV band to near-band-edge emission from the $Si/Si_{1-x}Ge_x$ superlattice. Thus, this band could be responsible for the hole (H) and electron (E) resonances both observed as luminescence-enhancing signals in these ODMR studies. A type-II near-band-edge recombination can be suggested since the anisotropic resonance (H) arises from holes confined in the SiGe layers and the feature labeled E has a g value that is consistent with an association to either electrons or shallow donors located in the Si layers. However, a type-I recombination mechanism cannot be ruled out. Finally, the near-band-edge PL may involve essentially unconfined electrons with a large wave-function extent since the conduction-band offset is predicted to be small.

In summary, ODMR of photoluminescence from a $Si/Si_{1-x}Ge_x$ superlattice grown on (001)Si has been performed for the first time. The work demonstrates the potential of ODMR to provide detailed information on the nature of the optical properties, electronic band structure, and the presence of native defects in this system. This study clearly confirms that the highest hole subband in the strained SiGe layers is derived from the $J_z=\pm\frac{3}{2}$ valence band. In addition, the results demonstrate that part of the emission originates from the superlattice region in these structures. Further studies of the recombination processes in this system are in progress.

J.M.T. is a National Research Council–NRL Resident Research Associate.

[1]For a review, see G. C. Osbourn, P. L. Gourley, I. J. Fritz, R. M. Biefeld, L. R. Dawson, and T. E. Zipperian, in *Semiconductors and Semimetals,* edited by R. Dingle (Academic, Orlando, 1988), Vol. 24, p. 459.

[2]D. V. Lang, R. People, J. C. Bean, and A. M. Sergent, Appl. Phys. Lett. **47**, 1333 (1985).

[3]T. P. Pearsall, F. H. Pollak, J. C. Bean, and R. Hull, Phys. Rev. B **33**, 6821 (1986).

[4]R. Zachai, K. Eberl, G. Abstreiter, E. Kasper, and H. Kibbel, Phys. Rev. Lett. **64**, 1055 (1990).

[5]H. Okumura, K. Miki, S. Misawa, K. Sakamato, and S. Yoshida, Jpn, J. Appl. Phys. **28**, L1893 (1989).

[6]E. A. Montie, G. F. A. van de Walle, D. J. Gravesteijn, A. A. van Gorkum, and C. W. T. Bulle-Lieuwma, Appl. Phys. Lett. **56**, 340 (1990).

[7]See, for example, K. B. Wong, M. Jaros, I. Morrison, and J. P. Hagon, Phys. Rev. Lett. **60**, 2221 (1988); S. Satpathy, R. M. Martin, and C. G. van de Walle, Phys. Rev. B **38**, 13227 (1988); S. Froyen, D. M. Wood, and A. Zunger, Phys. Rev. B **37**, 6893 (1988).

[8]R. People, J. C. Bean, D. V. Lang, A. M. Sergent, H. L. Stormer, K. W. Wecht, R. T. Lynch, and K. Baldwin, Appl. Phys. Lett. **45**, 1231 (1984).

[9]R. Braunstein, A. R. Moore, and F. Herman, Phys. Rev. **109**, 695 (1958).

[10]R. People, Phys. Rev. B **32**, 1405 (1985).

[11]G. Dresselhaus, A. F. Kip, and C. Kittel, Phys. Rev. **98**, 369 (1955).

[12]M. H. Brodsky and R. S. Title, Phys. Rev. Lett. **23**, 581 (1969).

[13]T. Shimizu, M. Kumeda, and Y. Kiriyama, Solid State Commun. **37**, 699 (1981).

[14]G. E. Pake and T. L. Estle, *The Physical Principles of Electron Paramagnetic Resonance* (Benjamin, Reading, MA, 1973).

[15]J. L. Patel, J. E. Nicholls, and J. J. Davies, J. Phys. C **14**, 1339 (1981).

[16]H. W. van Kesteren, E. C. Cosman, and W. A. J. A. van der Poel, Phys. Rev. B **41**, 5283 (1990).

[17]G. Feher, Phys. Rev. **114**, 1219 (1959).