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Room-temperature photoluminescence of $Ge_mSi_nGe_m$ structures

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Photoluminescence of pseudomorphic Ge wells grown by conventional molecular beam epitaxy on Si substrate is studied. The samples consist of *p*-type doped $Ge_m-Si_n-Ge_m$ structures embedded in a $Si_{1-x}Ge_x$ alloy. The luminescence lines shift to lower energy with increasing *m*, the observed band gap agrees with subband calculation based on an effective mass approximation. The temperature stability of the luminescence depends on *m*. In the case of $m=4$ the luminescence persists up to room temperature with only small reduction in intensity. The activation energies determined from the exponential drop of luminescence intensity agree with band discontinuities in the sample structures. © *1995 American Institute of Physics.*

Advances in growth techniques have led to improved optical properties of Si/Ge heterostructures. Intensive photoluminescence (PL) and electroluminescence from pseudomorphic alloy quantum wells and short period superlattices (SL) have been reported by several groups.[1] For short period SL the main concern has been the theoretically predicted enhancement of the optical matrix elements for the fundamental interband transitions. Despite the observation of rather strong luminescence in SLs at low temperatures,[2,3] it is still not clear, if this is caused by zone folding or just by symmetry braking due to the presence of the Si–Ge interfaces. Simpler structures which consist of thin $Ge_m-Si_n-Ge_m$ layers on different buffers have been suggested, for which also enhanced optical transition matrix elements are expected.[4] Luminescence of thin Ge layers (2 monolayers) grown pseudomorphically on Si was already demonstrated by Engvall *et al.*[5] Common to both, $Si_{1-x}Ge_x$ quantum wells and Si_mGe_n superlattices, is the quite strong drop of luminescence intensity with increasing temperature. If luminescence below the Si band gap was observed at room temperature, then it often included a defect related luminescence.[6,7] Recently, Fukatsu *et al.* demonstrated PL of deep SiGe alloy quantum wells at room temperature.[8] In this letter we report on strong PL of $Ge_mSi_{20}Ge_m$ structures embedded in a SiGe alloy. The band gap for different Ge well thicknesses is compared to subband calculations. The luminescence attributed to the Ge wells persists up to room temperature with only small reduction of the intensity.

The basic structure of the samples is shown in Fig. 1(a). Two *m* monolayers thick Ge wells are separated by 20 atomic planes Si. This $Ge_m-Si_{20}-Ge_m$ structure is embedded symmetrically (B2942-B2975) or asymmetrically (B2817) in a $Si_{1-x}Ge_x$ alloy matrix with a thickness of 10 nm. The layer sequence is repeated ten times with 40–50 nm thick Si layers in between to ensure pseudomorphic growth. The Ge thickness was 2, 3, or 4 monolayers thus approaching the critical thickness of pseudomorphically strained Ge on Si.[9] The whole sequence of quantum well layers is *p*-type doped with boron in the range of $10^{18}-10^{19}$ cm^{-3}. The doping is increased within the alloy and the wells by a factor of 2. We have used Sb as a surfactant to achieve sharp interfaces of the thin Ge layers. Incorporation of Sb leads to partial compensation of the B acceptors. The top layer was *n*-type doped

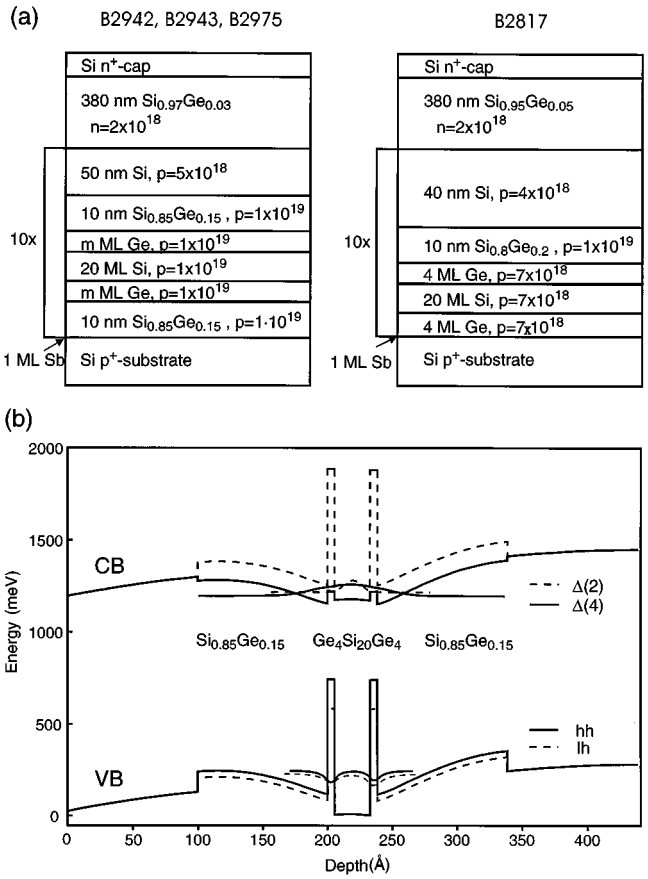

FIG. 1. (a) Structure of the samples: ten periods of $Ge_mSi_{20}Ge_m$ layers embedded symmetrically or asymmetrically in a $Si_{1-x}Ge_x$ alloy; (b) calculated band scheme for $m=4$ and symmetric cladding layers.

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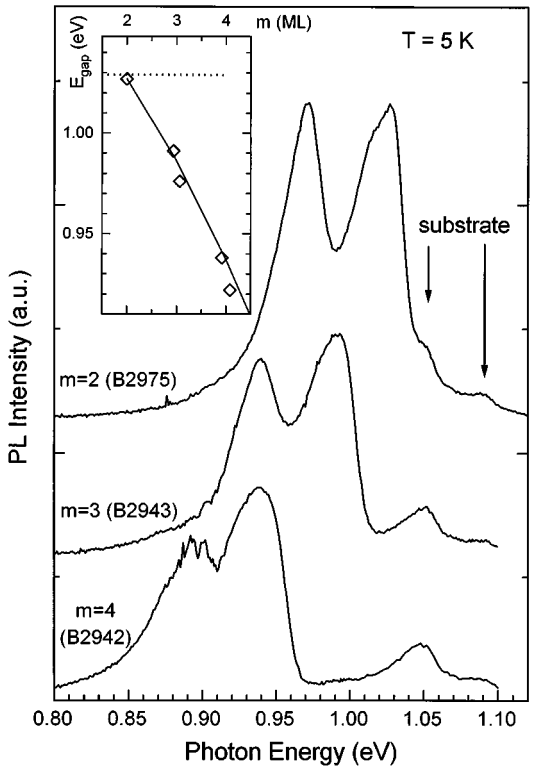

FIG. 2. PL of $Ge_mSi_{20}Ge_m$ structures for $m=2$, 3, and 4 at 5 K, in the inset the energetic position of the NP lines ($\diamond$) are compared to the calculated band gap of the $Ge_mSi_{20}Ge_m$ structures (solid line); the band gap of the embedding $Si_{0.85}Ge_{0.15}$ alloy is indicated by the dotted line.

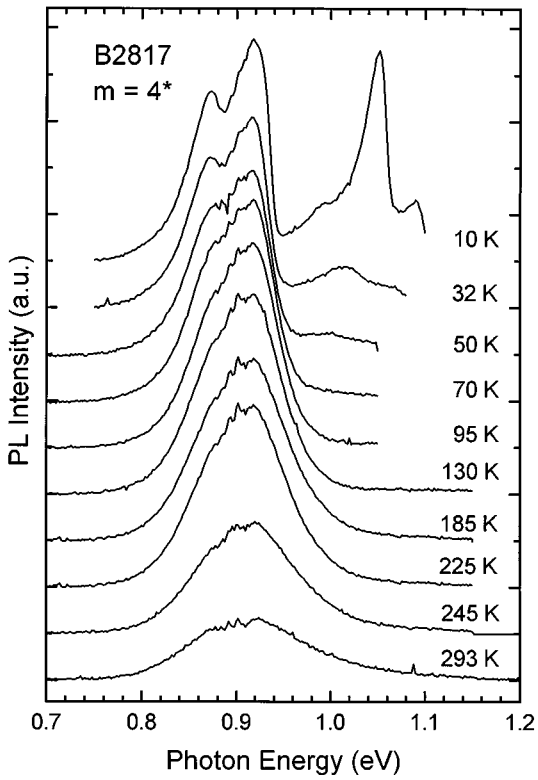

FIG. 3. PL of the $Ge_4Si_{20}Ge_4$ structure B2817 at various temperatures.

to form a *p-n* junction. Dopant concentrations and Ge contents in the alloy were measured by secondary ion mass spectroscopy (SIMS). Layer thicknesses were determined from x-ray diffraction measurements and transmission electron microscopy (TEM) pictures. Excellent structural quality of the samples has been achieved.

We have modeled the expected band structure of the samples by self-consistent subband calculations based on the valence band offsets given in Ref. 10. Effective masses were determined from interpolation of the Kohn–Luttinger parameters for Si and Ge.[11] The result for the sample with $m=4$ is shown in Fig. 1(b). The fundamental energy gap in an undoped structure is determined by the confined heavy hole (hh) states in the Ge wells and the four-fold degenerate in plane conduction band minima (Δ_4) in the SiGe alloy. The *p*-type doping induces a band bending which tends to localize the electrons in the $Ge_mSi_nGe_m$ layers. At sufficient high carrier concentrations the twofold degenerate (Δ_2) minima with the heavy mass normal to the interfaces are expected to form the energetically lowest conduction band state. Using the measured Sb and B concentrations the expected turnover of the Δ_4 and Δ_2 conduction band minima is just not completed, as can be seen in Fig. 1(b). The whole structure is part of the depletion region of the *p-n* junction inducing an overall band bending, which is also taken into account in this calculation. The effect on the electronic energy levels in the wells due to the built in electric field from the *p-n* junction is, however, negligible.

In Fig. 2 the PL spectra of pseudomorphic $Ge_mSi_{20}Ge_m$ structures with $m=2$, 3 and 4 are plotted. The luminescence signal at 5 K shows two prominent lines, which shift to lower energy with increasing Ge well thickness. The two weak peaks at 1.05 and 1.09 eV which do not depend on *m*, originate from the doped Si substrate. With increasing *m* the separation of the two intense lines decreases and the peaks are broadening. The Ge well thickness *m* is the only structural parameter changing in this series of samples. The lines due to the Ge wells correspond to no phonon (NP) line and TO replica. In the inset of Fig. 2 the energies of the NP lines are compared to the band gap calculation. The observed band gaps agree rather well with the calculated band gaps (full curve). In the case of $m=2$ the energy gap is close to the gap of the $Si_{0.85}Ge_{0.15}$ alloy. Therefore, the PL lines observed for sample B2975 may originate both from, the $Si_{0.85}Ge_{0.15}$ alloy and the embedded $Ge_2Si_{20}Ge_2$ structure. The band gap of a $Si_{0.85}Ge_{0.15}$ alloy is indicated by a dotted line in the inset of Fig. 2 The decreasing splitting of the NP line and the TO replica is due to the increasing influence of the Si–Ge and Ge–Ge phonon modes with increasing Ge layer thickness. Similar effects have been observed in SiGe alloys with increasing Ge content.[12]

In Fig. 3 the PL spectra of a $Ge_mSi_{20}Ge_m$ structure with $m=4$ are shown for various temperatures. The total intensity of the PL is only slightly decreasing up to room temperature. The substrate related luminescence disappears above 50 K. On the contrary the luminescence intensity of the $Ge_4Si_{20}Ge_4$ quantum well layer of sample B2817 first increases and reaches a maximum at 185 K followed by a strong decrease. Even at room temperature however, the intensity is only reduced by a factor of 2 compared to low

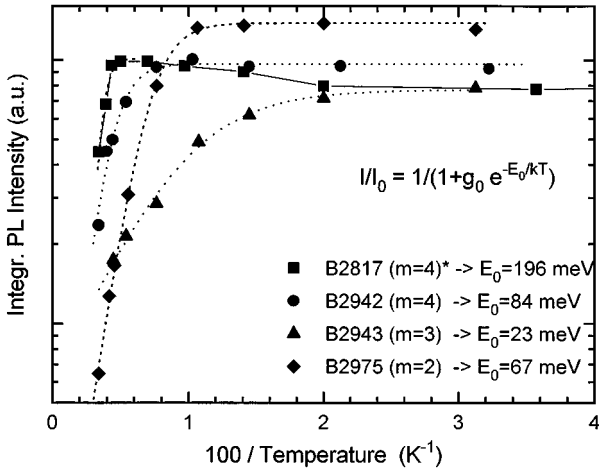

FIG. 4. Temperature dependence of the integrated Ge well intensity for different well widths.

temperature. In Fig. 4 the temperature dependence of the integrated luminescence originating from the Ge wells is shown for different well widths. It is interesting to note that the activation energies of the PL drop with temperature is strongly dependent on the well widths and the composition of the cladding layers. This results, for example, in the fact that only the thick wells ($m=4$) exhibit luminescence at room temperature. The drop in luminescence intensity with increasing temperature is stronger for sample B2942, which also contains Ge wells with 4 monolayers, embedded however in different cladding layers. For the samples with thinner Ge wells ($m=3$ and $m=2$) the luminescence from the quantum wells decays more rapidly with increasing temperature. The remaining signals at room temperature are shifted upwards in energy and correspond mainly to luminescence from the Si substrate or to the Si and SiGe cladding layers. Consequently, the carriers are no longer confined in the Ge layers at room temperature.

Since the thicker wells show luminescence at higher temperatures than the thinner wells, it is reasonable to assume that the intensity drop is mainly due to thermal activation of the carriers out of the quantum wells. Making this assumption, we can estimate the confinement energies from the decrease of the luminescence intensity with increasing temperature. The activation energies E_a obtained by a fit to the exponential drop of the integrated luminescence intensity[13] are listed in Fig. 4. The largest activation energy is observed for sample B2817. This sample differs from the others in a way that the cladding layers are asymmetric, SiGe towards to *n*-doped side of the *pn* junction and Si towards the *p*-doped side. Therefore, the barrier for the holes is increased from the Ge wells to the *p*-side of the *pn* junction. The activation energy found for B2817 corresponds to the band gap difference between Ge well states and Si rather than the discontinuity to the SiGe alloy. In the samples with symmetrical alloy layers the barrier is accordingly lower. The values of E_a determined for B2942 ($m=4$) and B2943 ($m=3$) are in reasonable agreement with the band discontinuities between the Ge well states and the embedding SiGe alloy. For sample B2975 containing only two monolayers of Ge, the hole states are very close to edges of the alloy barrier. Therefore, we believe the band discontinuity giving rise to the activation energy of 67 meV could be at the interface of the alloy to the Si layers.

In conclusion photoluminescence of thin Ge wells for various well widths has been observed. The energetic positions of the NP lines agree reasonably with the calculated band gap. The luminescence of the $Ge_mSi_{20}Ge_m$ structures persists up to room temperature with only small reduction of the intensity, if the wells are sufficiently thick ($m=4$). The activation energies found for the PL drop with increasing temperature as discussed in terms of band discontinuities. The samples also show electroluminescence, which will be published in detail elsewhere.

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