Photoluminescence in Short-Period Si/Ge Strained-Layer Superlattices

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Photoluminescence has been observed in the energy range 0.7 to 0.9 eV in short-period Si/Ge strained-layer superlattices grown on Si(100) and Ge(100) substrates. The luminescence is strongly influenced by period, layer-thickness ratio, and strain distribution. The experimental results are in good agreement with the expected fundamental energy gaps of the superlattices as calculated with a Kronig-Penney-type model.

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Recent developments in low-temperature molecular-beam epitaxy[1] allow the growth of high-quality Si/Ge strained-layer superlattices (SLS's) on both Si and Ge substrates.[2-4] The band structure is strongly influenced by strain distribution, layer-thickness ratio, and period. First optical experiments with evidence for new band gaps were published in the past few years.[5-7] Under certain conditions, Brillouin-zone folding effects are expected to create a quasidirect band gap in a Si/Ge SLS. This was first proposed by Gnutzmann and Clausecker[8] using simplified assumptions. The early ideas were the basis of extensive discussions and band-structure calculations of Si/Ge superlattices by various groups in recent years.[9-15] According to present knowledge a quasidirect energy gap with the lowest optical transition dipole allowed is only expected when the Si layers are strained and for periods of only a few monolayers (ML). Recently, we have observed photoluminescence from a strain symmetrized Si/Ge SLS with period of 10 ML grown on Si(100).[16] In this Letter we report on photoluminescence properties of various Si_mGe_n SLS's [(m ML)Si/(n ML)Ge] differing in period, individual layer thickness, and strain distribution. The results are discussed with respect to strain and superlattice effects by calculating the superlattice energy bands with a Kronig-Penney-type model.

The samples consist of an alternating sequence of pure Si and Ge layers grown on Si(100) and Ge(100) substrates at substrate temperatures of about 350 °C. The periodic structures have an overall thickness of about 200 nm. On the Si substrate the strain was adjusted by growing the SLS's pseudomorphically on different partially relaxed buffer layers (SiGe alloy and pure Ge) giving different intermediate lateral lattice constants for the superlattices (see Ref. 3). On the Ge substrate the strain was set by the degree of relaxation of the whole superlattice structure controlled by *in situ* LEED investigations (see Ref. 4). Some of the investigated structures have an almost symmetric strain distribution between the Si and Ge layers (layer thickness times absolute value of strain is constant). It should be noted that despite large efforts to improve the quality of the intermediate buffer layers,[17] there still exist a considerable amount of misfit dislocations in the SLS's.

Figure 1 shows typical photoluminescence of Si_3Ge_2, Si_6Ge_4, and $Si_{12}Ge_8$ superlattices grown on the Si substrate with an almost symmetric strain distribution (lateral strain in Si: $\epsilon_{\parallel}^{Si} \approx 1.4\%$). The small sharp line at about 1.1 eV arises from the Si substrate. By far the strongest luminescence originates from the 10-ML period Si_6Ge_4 superlattice at about 0.84 eV. The peak position of this signal is shifted to higher energies by approximately 25 meV with increasing excitation power

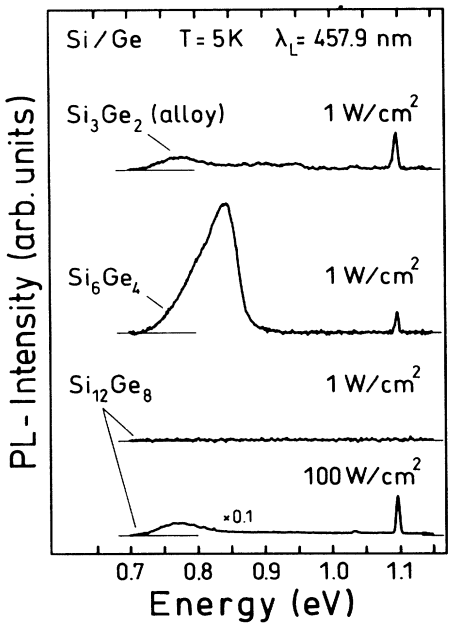

FIG. 1. Photoluminescence of various symmetrically strained Si_mGe_n superlattices grown on Si(100) substrate with periods of 5, 10, and 20 ML, common layer-thickness ratio $m/n = 1.5$, and biaxial strain $\epsilon_{\parallel}^{Si} \approx 1.4\%$ and $\epsilon_{\parallel}^{Ge} \approx -2.7\%$. The Si_3Ge_2 structures has a more alloylike behavior.

density from 0.1 to 100 W/cm^2.[16] The Si_3Ge_2 sample exhibits much broader luminescence below 1 eV with intensities at least 1 order of magnitude weaker. Similar weak features are also observed from a corresponding SiGe alloy reference sample. From the 20-ML period $Si_{12}Ge_8$ SLS no luminescence is observed in the investigated energy region for small excitation power density (1 W/cm^2). A weak signal at about 0.77 eV is observed only for high-excitation power density (100 W/cm^2). Also in the case of high-excitation power the peak intensity of the Si_6Ge_4 SLS luminescence is 10 to 20 times stronger than the low-energy signals from the other samples. The weak luminescence features from these reference samples are probably caused by recombination at defects (dislocations or impurities). In order to relate the strong SLS luminescence of the Si_6Ge_4 sample to the new superlattice band structure we have investigated several 10-ML period samples with different lateral lattice constants and consequently different strain distribution between the Si and Ge layers. It turns out that the luminescence peak energy is decreasing with increasing strain in the Si layers. The peak intensity remains considerably stronger than the broad signals of the reference samples. Preliminary results have been presented recently.[18]

In order to understand the strong influence of strain and period on the band structure of Si/Ge SLS's we have calculated the band structure in the envelope-function approach (Kronig-Penney–type model) as, for example, described in Ref. 19. The displacement of the atoms from their intrinsic positions leads to significant changes of the band gaps and offsets in the layered structure.[20,21] The band alignments in Si/Ge SLS's are calculated by means of linear deformation potential theory combined with band-offset values obtained by van de Walle and Martin.[22] Both the band edges (dashed and dash-dotted lines) and the minibands (hatched regions) obtained from these calculations for a Si_6Ge_4 superlattice are shown in Fig. 2(a) as a function of strain in Si. The zero energy is chosen as the heavy-hole band edge in the Ge layers. Strain-induced splitting of the sixfold-degenerated Δ conduction-band (CB) minima and the heavy- and light-hole (hh,lh) valence-band (VB) maxima lead to a staggered band lineup for all possible strain distributions. The CB well is formed in the Si layers, whereas the top of the VB well is highest in the Ge layers. The $\Delta_\perp$ ($\Delta_\parallel$) well and the corresponding lowest miniband $\Delta_\perp^1$ ($\Delta_\parallel^1$) is shifted to lower (higher) energies with more strain in the Si layers. Intervalley interactions have been neglected in the calculations. In (100)-oriented Si/Ge SLS's a quasidirect energy gap is expected only if the states originating from the twofold-degenerate $\Delta_\perp$ minima along the growth direction are lower in energy than the fourfold-degenerate in-plane $\Delta_\parallel$ states. This requires a tensile strain of about 1% in Si [see Fig. 2(a)]. Therefore no quasidirect energy gap is expected in Si/Ge SLS's grown lattice matched to Si. The $\Delta_\parallel$ states are

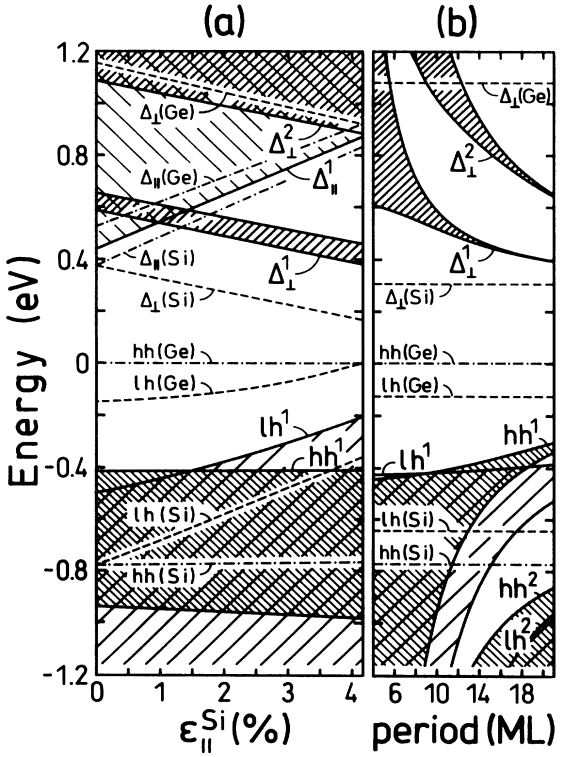

FIG. 2. Band edges (dashed and dash-dotted lines) in the individual layers and superlattice states (hatched regions) calculated with a Kronig-Penney–type model: (a) for a Si_6Ge_4 superlattice as a function of biaxial strain in the Si layers; (b) for a Si_mGe_n superlattice with $m/n = 3/2$ and almost symmetric strain distributor ($\epsilon_\parallel^{Si} = 1.4\%$) as a function of period.

delocalized, whereas the $\Delta_\perp$ ground states are more localized in the Si layers (miniband width ≈ 70 meV). In the valence band the hh and lh states are delocalized. Because of the staggered band lineup delocalization of at least one of the corresponding states is necessary to achieve large overlap of the wave functions and a strong optical transition probability. For sufficient high strain in Si the lh-miniband edge (lh^1) is highest in energy. The effective electron masses are expected to be independent of strain, whereas for the holes the strain dependence has to be taken into account.[23] The strain-induced coupling of the $\frac{3}{2}, \frac{1}{2}$ (lh) states with the $\frac{1}{2}, \frac{1}{2}$ (spin-orbit–split-off states) is expected to lead to a decrease (increase) of lh confinement mass in the Si (Ge) layers from about $0.2m_0$ ($0.05m_0$) in the unstrained case to about $0.18m_0$ ($0.14m_0$) in the highest strain case, respectively.

In Fig. 3 the lower band gaps between the miniband edges are shown as a function of strain in Si for a Si_6Ge_4 SLS (solid lines) and a Si_4Ge_6 SLS (dashed lines). For sufficient high strain in Si the fundamental band gap is determined by the energy difference between the zone-folded $\Delta_\perp$ and the lh states. With more strain in Si the band gap is reduced from about 0.9 eV ($\epsilon_\parallel^{Si} \approx 1.4\%$) to

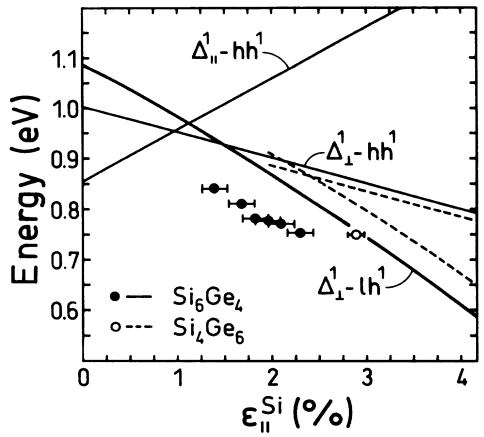

FIG. 3. Photoluminescence peak energies of Si_6Ge_4 superlattices (dots) and a Si_4Ge_6 superlattice (open circle) compared with calculated values of the relevant band gaps for Si_6Ge_4 (solid lines) and Si_4Ge_6 (dashed lines) as a function of biaxial strain in the Si layers.

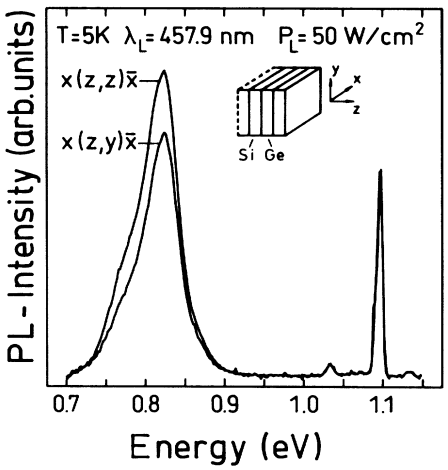

FIG. 4. Polarization dependence of the photoluminescence of a Si_6Ge_4 superlattice with biaxial strain $\epsilon^{Si}_{\parallel} \approx 1.4\%$ and $\epsilon^{Ge}_{\parallel} \approx -2.7\%$ (measured in backscattering geometry from the edge of the sample; the spectra are normalized to the polarization-dependent efficiency of the grating, which leads to identical intensities of the Si luminescence peaks).

about 0.6 eV ($\epsilon^{Si}_{\parallel} \approx 4.2\%$). An increase of the Ge layer thickness in a 10-ML period SLS shifts the lh gap to higher energies and the hh gap slightly to lower energies (see Si_4Ge_6). The essential features obtained from this simple model are in surprisingly good agreement with more sophisticated band-structure calculations (see, for example, Ref. 13).

The measured photoluminescence peak energies for the various 10-ML period samples are also shown in Fig. 3. Both the layer thicknesses and the strain distribution were determined by a careful analysis of Raman experiments (energy shift of the folded acoustic- and the longitudinal-optical modes).[3] The parameters of the Ge-based structure were determined in addition to LEED and TEM investigations.[4,24] The layer thicknesses agree well with the expected values. The estimated uncertainty in the strain values is given by the error bars in Fig. 3. As expected from theory the peak shifts to lower energies with more strain in the Si layers. The luminescence peak energies are about 100 meV lower than the corresponding calculated band gaps. This discrepancy is, however, understandable taking into account the uncertainty of the VB offsets, deformation potentials, and valence-band masses used in the calculation. It is also expected that strain and thickness fluctuations lower the optical transition energies and further on cause a rather broad luminescence signal. A low-energy broadening of the luminescence (see Fig. 1) is observed in structures with high Sb doping. The major features of the experimental results are well described by the theory. We therefore believe that the observed luminescence is basically related to transitions from the zone-folded $\Delta_\perp$ states to the highest valence-band states, which are the light-hole states for high enough strain.

To obtain more information on the nature of the SLS photoluminescence we have performed experiments in backscattering geometry from the polished edge of the layered structure (see Fig. 4). The luminescence from the Si_6Ge_4 SLS ($\epsilon^{Si}_{\parallel} \approx 1.4\%$) polarized parallel to the layers $[x(z,y)\bar{x}]$ is 20% weaker than polarized perpendicular to the layers $[x(z,z)\bar{x}]$. As expected the luminescence from the Si substrate is not polarization dependent. Transitions to lh VB states are expected to cause polarized luminescence perpendicular to the layers $[x(z,z)\bar{x}]$. The calculated crossover between hh and lh states is, however, close to the strain value of the studied sample. This might explain the relatively weak polarization dependence observed in the experiments. The SLS luminescence peak energy is shifted to lower energies compared with the results obtained in a front surface geometry (see Fig. 1). The laser spot (diameter ≈ 0.1 mm) was focused on the edge of the sample essentially stripping the sample surface. We believe that in the edge geometry the excited carrier density is much smaller than for a front surface excitation, where a blueshift with increasing optical-induced carrier density was observed.[16]

The dependence of the superlattice states on period is given in Fig. 2(b) for a layer-thickness ratio of 6(Si)/4(Ge) and 1.4% strain in the Si layers. As expected both the CB and the VB ground states are more localized in the corresponding layers for larger periods (electrons in Si layers, holes in Ge layers). Even for a period of 20 ML the $\Delta_\perp$ ground state has a miniband width of less than 1 meV. In the VB the more localized hh states become dominant for the effective superlattice band gap. The spatial separation of the carriers decreases the optical transition probability drastically. This is reflected in the experiments where strong luminescence has been observed so far for only periods of the order of 10 ML.

In summary, strong photoluminescence in Si/Ge strained-layer superlattices is observed in the energy range 0.7 to 0.9 eV. The transition energies depend critically on strain distribution and layer thickness within the 10-ML periods. The strongest luminescence is obtained in symmetrically strained structures. The low-energy superlattice states have been calculated with a Kronig-Penney-type model. The strain dependence of the photoluminescence is in good agreement; the absolute energy in reasonable agreement with the theoretically expected transitions from the folded Δ conduction-band minimum to the valence-band maxima. Consequently, the results reported here support the idea of a quasidirect energy gap in short-period Si/Ge superlattices.

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