Photoluminescence of the two-dimensional hole gas in p-type δ-doped Si layers

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The radiative recombination processes related to the boron-δ-doping of Si layers are studied by means of photoluminescence (PL) spectroscopy. New broad asymmetric PL bands below the band edge excitonic emissions are shown to be characteristic for p-type modulation doping. By studying the dependence of the PL properties on structure parameters, such as doping level and growth temperature, and on the experimental conditions the mechanisms of the radiative recombination are analyzed. The PL revealed is argued to be related to the recombination between the two-dimensional hole gas confined in the doping-induced notch potential and photocreated electrons.

The realization of modulation doping, especially for Si-based structures represents an important step in semiconductor technology.[1] Using the concept of modulation or selective doping it has been possible to separate charge carriers from dopants and, thus, to reach greatly enhanced carrier mobilities.[1–4] Moreover, modulation doping is known as an alternative way to achieve a quantum well (QW) structure without a heterojunction,[1,5] i.e., with high interface quality. The previous studies of modulation-doped Si thin films have been mostly focused on magnetotransport phenomena[2–4] and far-infrared absorption measurements.[5,6] Very little has been done by photoluminescence (PL) spectroscopy despite the known capability of this technique for direct investigations of the optical and electronic properties of two-dimensional (2D) carriers, demonstrated previously in III-V heterostructures.[7–9] The main reason for the so far limited PL studies is the difficulty to satisfy simultaneously two contradictory requirements, i.e., to secure a sharp dopant distribution by using interrupted growth,[10,11] low-temperature growth[12] or ion-beaming doping,[13] and at the same time to obtain a reasonable high radiative efficiency suitable for optical studies.

In this paper we shall show that p-type modulation doping strongly affects the radiative recombination processes in Si thin films grown by molecular beam epitaxy (MBE). The properties of new asymmetric PL bands, appearing due to the modulation doping, are studied as a function of growth parameters, such as growth temperature and doping concentration, and experimental conditions. The PL observed is discussed in terms of radiative transitions involving a 2D hole gas (2DHG), formed as a result of the doping. The participation of the 2DHG in the recombination process is confirmed by varying the doping level, and by hydrogen passivation, where a complete quenching of the new PL bands with decreasing doping concentration below the degenerate limit was observed.

Samples investigated were grown on phosphorous-doped (100)-oriented Si substrates in a Balzers UMS-630 MBE system. Boron doping was achieved by sublimation of elemental B from a high-temperature effusion cell. The growth temperature was about 420 °C. The investigated structures consist of two periods of heavily boron-δ-doped regions (with a sheet concentration ranging from 2×10^{12} cm^{-2} to 5×10^{13} cm^{-2}) separated by 1000–2000 Å undoped Si spacers. The dopant concentration and distribution were determined by secondary-ion-mass spectrometry (SIMS). The measured B profiles have a full width at half maximum $\leqslant$75 Å (limited by the SIMS depth resolution). The electrical activity of the B dopants was $\sim$100% according to Hall-effect measurements.

Photoluminescence was measured in a temperature range 2–77 K using the 514.5 nm line of an Ar^+-ion laser as an excitation source. The luminescence was dispersed with a SPEX 0.85 m double-grating monochromator equipped with a liquid-nitrogen-cooled North Coast Ge detector. The PL signal was recorded with a conventional lock-in technique in phase with the frequency of a mechanical chopper. The spectra were not corrected for the response of the detection system.

Figure 1 represents the dependence of the PL spectra of the modulation-doped Si layers on the growth parameters, i.e., B doping concentration and growth temperature. All spectra in the near band gap region contain several luminescence lines originating from free excitons (FE) and phosphorous (P) bound excitons. The latter consists of the no-phonon (NP) line P^{NP} at 1.150 eV, the weak transverse-acoustic (TA) replica P^{TA}, and the intense transverse optical (TO) phonon-assisted transitions P^{TO}. The FE emission is, however, dominated by the TO-phonon replica FE^{TO}. The emission which appears at the low energy side of the P^{TO} line is due to recombination of electron-hole droplets (EHD).[14] All these emissions are related to the substrate and will not be discussed further in this report. In addition two relatively broad asymmetric PL bands (denoted as the BD band for boron δ doping—Fig. 1), corresponding to the weak TA (not labeled in the Fig. 1) and strong TO replicas, are observed below the shallow bound exciton emission. These bands appear only in δ-doped structures with the doping concentration exceeding $4-6\times10^{12}$ cm^{-2}—Figs. 1(b) and 1(c). The decrease of the B concentration below this limit, either due to the lower doping [Fig. 1(a)] or due to the post growth passivation of B acceptors by hydrogen [the dashed curve in Fig. 1(b)], causes complete quenching of the BD bands. The

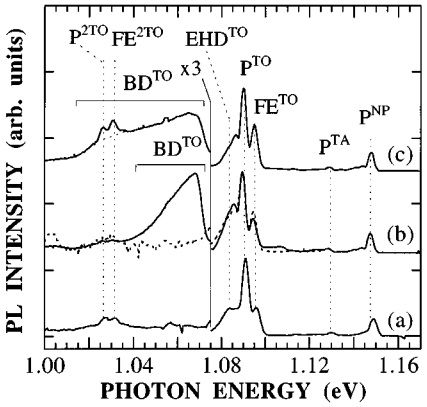

FIG. 1. Normalized photoluminescence spectra at 2 K from modulation-doped Si layers grown at 420 °C with B doping concentrations of 2×10^{12} cm^{-2} (a), 1×10^{13} cm^{-2} (b), and 5×10^{13} cm^{-2} (c). The spectrum of the hydrogen-passivated sample is shown by the dashed curve in (b). All spectra in the near band gap region contain substrate-related emissions originated from the free exciton (FE), phosphorous (P) bound exciton (BE) and electron hole droplets (EHD). The superscripts NP, TA and TO indicate the no-phonon transitions, transverse acoustic, and transverse optical phonon-assisted transitions, respectively. BD denotes transitions caused by the B δ doping.

width of the band increases with increasing doping level, i.e., it is about twice larger for the sample with the highest doping than for the 10^{13} cm^{-3} doping level—compare Figs. 1(b) and 1(c). The intensity of the BD bands with respect to the substrate-related emissions is slightly higher for the layers with intermediate doping [Fig. 1(b)]. This is attributed to an introduction by doping of strongly competing nonradiative defects,[15] as well as to enhanced Auger recombination due to a higher concentration of the 2DHG.

The properties of the PL bands are strongly dependent not only on the doping level as discussed above (Fig. 1), but also on the experimental conditions such as photo-excitation intensity and temperature. The PL spectra as a function of excitation density are shown in Fig. 2(a). (For simplicity we show below only the TO-assisted emission BD^{TO}, to avoid complications due to strong overlapping of the substrate-related PL.) With increasing photo-excitation density W, an enhancement of the PL intensity at the higher energy side of the spectrum is observed. This enhancement is followed by a blue shift of the PL maximum position with a further increasing excitation power. The magnitude of the shift under similar excitation conditions is found to be larger for lower doped structures, reaching up to 6 meV. A further increase in W causes a strong enhancement of the bulk-related EHD recombination at $\sim$1.080 eV overlapping with and eventually obscuring the BD PL bands. With an increasing temperature, on the other hand, the high-energy part of the PL quenches drastically and is no longer observed at temperatures higher than 8 K. However, the low-energy part of the PL emission can still be detected up to $\sim$30 K, as depicted in Fig. 2(b). All these experimental observations provide clear evidence that the BD band is composed of two overlapping components within the broad emission, with the low-energy one being rapidly saturated with increasing photoexcitation.

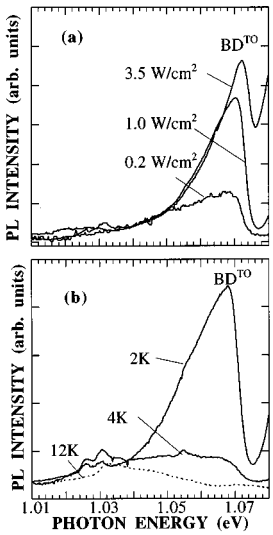

FIG. 2. (a) Excitation-dependent PL spectra at 2 K from the Si films with $[B]\sim1\times10^{13}$ cm^{-2} grown at 520 °C with photoexcitation $W=0.2$, 1.0, and 3.5 W/cm^2, respectively. (b) Temperature-dependent PL spectra measured for the same structure. The structure observed at $\sim$1.03 eV is related to FE^{2TO} and BE^{2TO} lines.

Similar but not identical emissions have been observed previously in uniformly boron-doped bulk silicon[16–18] and epitaxial films[19] with a doping level exceeding the degenerate limit. It should be pointed out that the PL detected in our

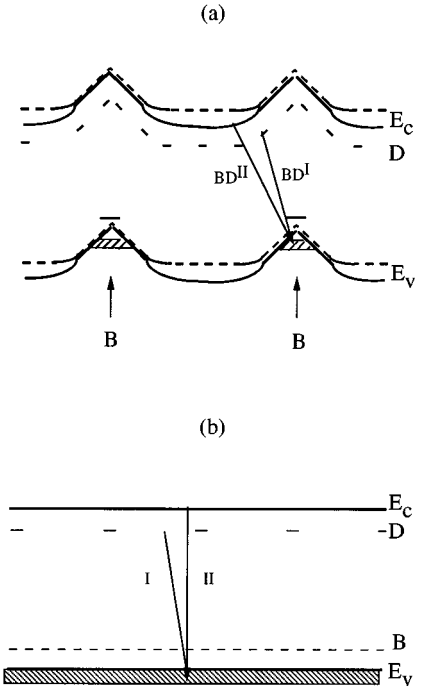

FIG. 3. Schematic band diagram of p-type δ-doped (a) and uniformly doped (b) silicon, both above the degenerate limit. Transitions labeled as I and II correspond to the recombination of the hole gas with electrons trapped by residual donors and free electrons, respectively. The solid and dashed lines in (a) correspond to the situation of low- and high-photoexcitation intensity, respectively. The donor levels for the high excitation conditions are not shown for clarity.

structures is shifted by 10–20 meV (depending on the doping level) towards lower energy as comparing with the uniform bulk doping. The space charge in the acceptor-doped regions is known to induce a notch potential well for holes leading to the formation of a 2DHG, as shown in Fig. 3. We thus attribute the PL observed to the radiative recombination of the 2DHG formed within the doped regions and nearby photocreated electrons. The width of the band gives a measure of the E_F position in the well, which is, e.g., $\sim$25 meV for Si layers with a doping level of 1×10^{13} cm^{-2} [Fig. 1(b)]. An increase of the doping level should enhance the filling of the well and will consequently induce a broadening of the 2D-related emission, in agreement with our experimental observations [Fig. 1(c)]. The requirement of the Fermi level line-up within the entire structure will cause a band bending in the vicinity of the doped spikes, thus creating a repulsive potential for photocreated electrons, as shown in Fig. 3(a). Consequently, the electrons and holes participating in the recombination will be confined in different regions of the charge-induced potential leading, in particular, to the observed shift towards lower energy of the PL relative to that from the uniformly doped bulk crystals—Fig. 3. It is, however, complicated to estimate the value of this shift because of the band gap renormalization effects, shown to be important for highly B-doped bulk Si.[15–17]

The two components of the PL emissions can be interpreted as arising from the recombination of the hole gas with electrons trapped by residual donors [the low-energy PL component, labeled as I in Fig. 3(a)] and with free electrons [the higher-energy component, labeled as II in Fig. 3(a)], as was previously proposed to explain a similar dependence of the PL spectra on the excitation intensity in heavily, uniformly doped bulk Si.[16–18] Due to a low concentration ($\sim10^{15}$ cm^{-3}) of the residual donors in our samples, a rapid saturation of the bound-to-free recombination with increasing excitation density and thus a dominance of the free-to-free recombination transitions in the PL spectrum are expected to occur.

The model proposed for the BD emissions implies that the PL spectra should shift towards the higher energies with an increasing photo-excitation, which is indeed observed in the experiments. Such a shift is partially attributed to the additional filling of the QW with photocreated holes. More importantly, the photogeneration of free carriers will also affect the potential distribution across the Si spacer by neutralization charged impurities, reducing the band bending under high excitation conditions. Such a band flattening will cause a shift of the PL to higher energy—Fig. 3(a). The shift is expected to be more pronounced for the lower doped structures, in agreement with experimental data.

As it was mentioned above, the potential confining the holes is repulsive for the photocreated electrons, see Fig. 3(a). Thus, the 2DHG and the electrons are separated in real space. This reduces the overlap of electron and hole wave functions and therefore the radiative recombination probability is expected to be low. The rather efficient 2D-related PL observed in our structures implies that the photocreated electrons are confined close enough to the doped region. In principle, such a confining potential could be created by the presence of a nearby doping spike, since the photocreated electrons will be localized between two notch potentials. However, the spatial separation between the doped regions in our samples is 1000–2000 Å, which is too large to ensure a strong overlap of the carrier wave functions. In addition, a PL enhancement rather than quenching with increasing temperature should be observed in this case due to the thermal activation of trapped photocreated electrons from the residual donors. This is, however, inconsistent with our experimental data [Fig. 2(b)]. We thus propose that the electrons are confined nearby the doping regions by a photo-induced potential created by the excess holes of the 2DHG. The expected depth of the confinement potential is in the order of a few meV[9] [not shown in Fig. 3(a)]. This explains the rapid thermal quenching of the high-energy PL component since the thermally activated release of the electrons from this potential will lead to an increasing spatial separation between the 2DHG and the free electrons and thus to a reduced recombination efficiency.

In summary, we have shown that p-type modulation doping strongly affects the radiative recombination processes in Si epilayers grown by the MBE technique. It is shown that the δ-doping-induced formation of a quasi-2D electronic system with the 2D hole gas confined in a space-charge-induced potential well gives rise to a broad asymmetric PL band, at 20–40 meV below the shallow bound exciton emissions. The observed strong thermal quenching of this PL band suggests that the photocreated electrons are localized near the doping spike with a rather shallow (1–2 meV) photoinduced potential.

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