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Band alignments and photon-induced carrier transfer from wetting layers to Ge islands grown on Si(001)

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Temperature- and excitation-power-dependent photoluminescence measurements were carried out for the multilayer structure of Ge islands grown on a Si(001) substrate by gas-source molecular-beam epitaxy. When the excitation power increases from 10 to 400 mW, the photoluminescence peak from the Ge islands showed a large linear blueshift of 34 meV while that of the wetting layers did not change much. These two different power dependences are explained in terms of type-II and type-I band alignments for the islands and the wetting layers, respectively. When the sample temperature increased from 8 to 20 K, an anomalous increase of photoluminescence intensity for islands was accompanied by a rapid decrease of that from the wetting layers, implying that a large portion of photon-induced carriers in the wetting layer was transfered to the neighboring islands and the Si layer, respectively, thus resulting in an increase of photoluminescence intensity of the islands.
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Recently, many studies have been done on the growth mechanism, electrical and optical properties of Ge islands (ID) embedded in Si. The growth behavior and resulting structure of the islands influenced by the wetting layers (WLs) has been investigated.[1,2] Although photoluminescence (PL) from Ge islands has also been widely studied,[1–8] little has been done on the correlation between PL from the islands and the wetting layers.[7,8] In this letter, both excitation power and temperature-dependent PL spectra of Ge islands and of wetting layers were measured with a power level from 10 to 400 mW and a temperature range from 8 to 300 K. Different power-dependent behaviors of the PL peak position were observed for the wetting layers and islands. Besides, the PL intensity from the islands increased significantly as the temperature increased from 8 to 20 K, the transfer process of photon-induced carriers in the wetting layers to the islands was evidenced at this temperature range.

The sample was grown on a Si(001) substrate by gas-source molecular-beam epitaxy (MBE) with a Si_2H_6 gas source and a Ge effusion cell. Ten layers of Ge islands separated by Si spacer layers were grown at the temperature of 575 °C. The thicknesses of the Ge island layer and the Si spacer layer were 1.6 and 50 nm, respectively. The PL measurements were performed by excitation of an Ar^+ laser and with a liquid-nitrogen-cooled Ge detector. The spot size of the laser on the sample was about 1 mm^2.

Figure 1 shows the PL spectra measured at 4.5 K with different excitation power levels. Apart from the peaks of the Si, the spectrum consists of two separate components which are characteristic of Ge wetting layer and Ge islands, respectively. The two main peaks located at 1007 and 949 meV are attributed to the NP_{WL} transition and its TO_{WL} phonon-assisted transitions of upper pseudomorphic wetting layers, while the two peaks denoted by NP_{WL1} and TO_{WL1} lines can be assigned to the NP transition and its TO replica in the first grown Ge wetting layer, as observed and correctly interpreted in Ref. 3. The energy difference between the NP_{WL} and TO_{WL} and between the NP_{WL1} and TO_{WL1} lines is 58 meV, which corresponds to the Si–Si optical phonon energy in Si.[4,9] The broad PL peak located around 0.83 eV was assigned to the PL from the island and it could be deconvoluted into two Gaussian line-shaped peaks at 824 and 866 meV, respectively, when the excitation power is 400 mW. The origin of these two peaks is still not clear. They might be attributed to either a bimodal island size distribution[1] or the

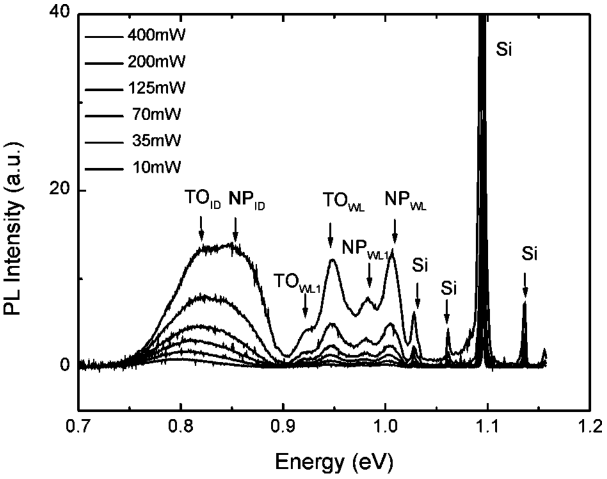

FIG. 1. PL spectra of Ge/Si (001) islands under different excitation power levels measured at 4.5 K. In addition to the PL peaks from Si, there are two separate components, which come from the islands and the wetting layer, respectively. The TO and NP PL lines originating from the first wetting layer and the upper wetting layer are indicated by TO_{WL1}, NP_{WL1}, TO_{WL}, and NP_{WL}, respectively. The PL band from the islands could be deconvoluted into two Gaussian line-shaped peaks which are indicated by TO_{ID} and NP_{ID}, respectively.

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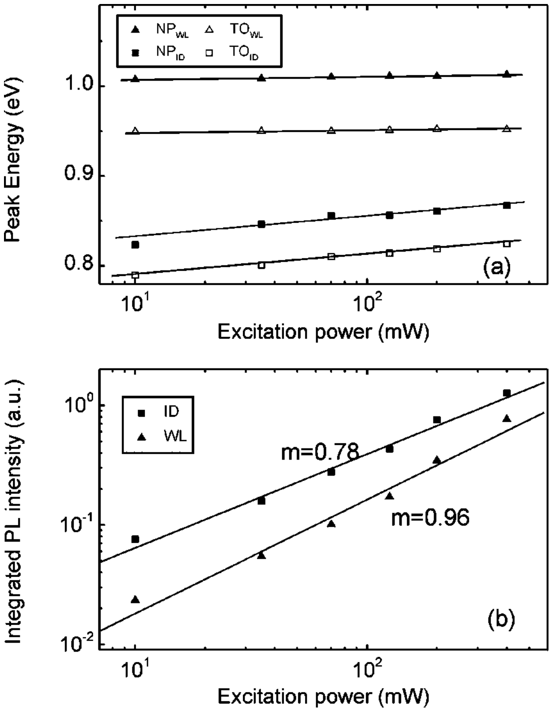

FIG. 2. Power dependence of PL peak energies (a) and integrated PL intensity (b) from the islands and the wetting layer. The peak energies from the islands show a blueshift with increasing excitation power while the peak energy from the wetting layer almost remains unchanged. This means the band alignment of the islands and the wetting layer are type-II and type-I, respectively. The different coefficients m of the power dependence of PL intensity ($I \propto P^m$), i.e., $m<1$ for the islands and $m \sim 1$ for the wetting layer, are found.

NP transition and TO replica of the Ge islands.[4–6] The TO mode may be $\mathrm{TO}_{\mathrm{Ge-Ge}}$ (Ref. 4) or $\mathrm{TO}_{\mathrm{Si-Ge}}$.[9,10]

Figure 2(a) shows the excitation power dependence of PL peak energies of the wetting layer ($\mathrm{TO}_{\mathrm{WL}}$ and $\mathrm{NP}_{\mathrm{WL}}$) and the Ge islands ($\mathrm{TO}_{\mathrm{ID}}$ and $\mathrm{NP}_{\mathrm{ID}}$). The $\mathrm{TO}_{\mathrm{ID}}$ and $\mathrm{NP}_{\mathrm{ID}}$ peaks of the islands show a large linear blueshift of 34 meV with increasing excitation power from 10 to 400 mW. The energy difference between them remains at 42 meV. The shift is comparable to a previous work reporting a blueshift value of 20 meV when the excitation power increased from 0.6 to 20 W/cm^2 for Ge nanostructures on a Si (118) substrate.[6] The blueshift of the PL band with the increase of excitation power suggests a type-II band. As the electrons and holes occupy two separate regions, a dipole layer is then formed due to the fact that the holes are confined in the Ge islands while electrons are confined outside. Then, a band bending will occur at the interfaces due to the Hartree potential. At high-excitation-power densities, more photon-induced electrons and holes will result in a higher Hartree potential, which will cause the electrons and holes to be in higher energies states, resulting in the blueshift of the PL band.[6,7,11] It is known that the band-filling effect could cause the PL blueshift with the increase of excitation power. However, it was calculated that in a type-II structure the line shift due to band filling is only several meV for general PL measurements and this effect is almost an order of magnitude smaller than the shifts induced by band bending.[12]

In contrast to the PL from Ge islands, the $\mathrm{TO}_{\mathrm{WL}}$ and $\mathrm{NP}_{\mathrm{WL}}$ peak positions of the wetting layers remain almost unchanged ($\sim$2 meV) when the excitation power increased. For this case, a type-I band alignment at the wetting layer/Si interface is more reasonable. Schmidt *et al.*[7] observed PL peak blueshifts for both Ge islands and wetting layers with the increase of excitation power and pointed out that both band alignments are type-II structures. In our results, the band alignments for Ge islands and wetting layers are type-II and type-I, respectively, and the power dependence of its PL intensity, as showed in Fig. 2(b), further supports the type-I band alignment at the wetting layer/Si interface. Different alignment types between our results and Ref. 7 may be attributed to the different Ge concentrations in Ge islands and wetting layers.

Figure 2(b) shows the power dependence of the integrated PL intensity from the Ge islands and the wetting layers. According to the formula $I \propto P^m$, where I represents the PL intensity and P the excitation power,[6] the coefficients m are found to be 0.96 and 0.78 for the PL from the islands and the wetting layer, respectively. The sublinear power dependence of the PL intensity of the islands is due to typical saturation effects for the type-II alignment. In a type-II alignment, the indirect excitons are first localized at the interfaces, and then they recombine. As the interface state density is limited, the PL quickly saturates.[6] For the wetting layer, there is no saturation as it is a type-I structure.

It is known that the band alignment of a strained $\mathrm{Si}_{1-x}\mathrm{Ge}_x/\mathrm{Si}$ heterostructure with higher Ge composition is type-II.[13] If there is no atomic intermixing at the Ge/Si interface, the wetting layer should be pure Ge, and then type-II band alignment is expected. However, first, atomic intermixing occurs during MBE growth even at low temperatures. High-resolution Rutherford backscattering spectroscopy studies showed that when 1.5 ML Ge was deposited on Si at 500 °C, the obtained Ge concentrations in the first four layers were 64.5%, 38%, 22.5%, and 11%,[14] indicating a significant Ge/Si intermixing during growth. Second, the formation of islands will introduce a strain into the Si substrate, and thus the alloying effect may be enhanced.[15] Due to atomic intermixing, the Ge islands were found to be $\mathrm{Si}_{0.45}\mathrm{Ge}_{0.55}$ alloy islands by using synchrotron radiation x-ray diffraction measurements in a previous work.[16] Likewise, theoretical calculations showed that the composition of the islands was not, in general, the same as the wetting layer;[17] a lower Ge content in the wetting layer than that in the islands was possible. In our case, the lower Ge content in the wetting layer might happen in our sample, thus resulting in a type-I band alignment at the wetting layer/Si interface.

Figure 3(a) shows the integrated intensities of PL from the islands and the wetting layer as a function of temperature. Interestingly, as the temperature increases, the PL intensity from the islands increases first in the temperature range of 8–20 K, and then decreases. At the same time, the PL from the wetting layer drops quickly and disappears at 40 K. Figure 3(b) shows the PL spectra measured at 8, 12, and 20 K, respectively. It is clearly seen that the anomalous increase of PL intensity from the islands is accompanied by a rapid decrease of PL intensity from the wetting layers, implying that a large portion of photon-induced electrons and holes in the wetting layers could be transferred to the islands rather than forming excitons in the wetting layers, then to radiatively recombine. Fukatsu *et al.*[8] observed a similar ex-

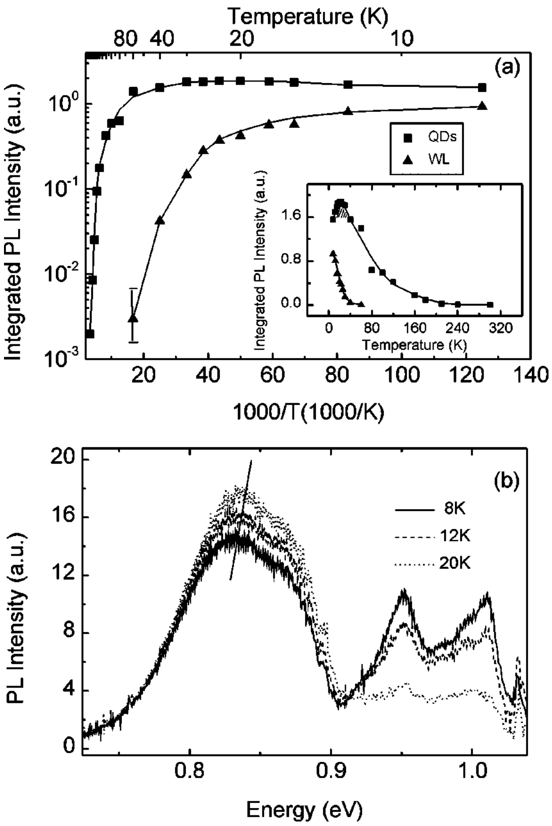

FIG. 3. (a) Temperature dependences of integrated PL intensities from the islands and the wetting layers. (b) PL spectra taken at 8, 12, and 20 K. It is clearly shown that the anomalous increase of the island PL intensity at the temperature of 8–20 K is accompanied by a rapid decrease of the wetting-layer PL intensity.

citon transfer from ''E dots'' (which is formed around the front Ge/Si interface) to ''S–K dots'' (which is the same as the Ge dots discussed here) around 20–50 K. However, in our case, the carrier transfer is from the wetting layer to the quantum dots because the rapidly decreased PL spectra have the typical characteristic of the wetting layer. Figure 4 illustrates the band alignments of the wetting layer and the Ge islands sandwiched by Si layers and shows the photon-induced carrier transfer process. Dashed arrows show the PL transition process in the wetting layer and the islands, respectively. For the wetting layer, when the temperature increases, holes and electrons which are previously trapped in the wetting layers at low temperatures could thermally be activated to move to the islands and the region near the islands, respectively, as shown in Fig. 4 (top). Thus, more holes will be trapped in the islands and attract more electrons to near the islands, resulting in an increase of PL intensity of the islands at higher temperatures. This photon-induced carrier transfer process is further supported by a slight PL blueshift from 8 to 20 K, as seen in Fig. 3(b). The reason for the slight blueshift at low temperature (8–40 K) is that more holes and electrons are transferred from the wetting layers to the islands and the regions near the islands. The resultant Hartree potential will become slightly higher, thus resulting in a blueshift of the corresponding PL peak for the islands, which is similar to the case of increasing excitation power as discussed before.

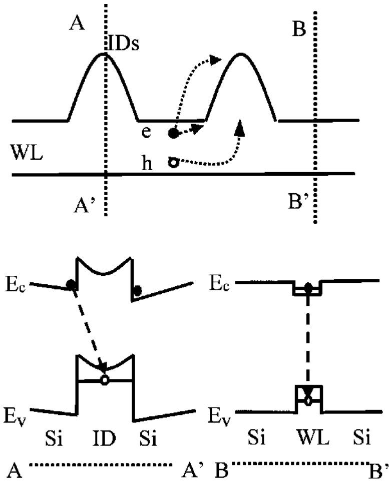

FIG. 4. Schematic diagram of the band alignments for the islands and the wetting layer (bottom). Carrier transfer process from the wetting layers to the islands is illustrated on top. Type-II and type-I band alignments are shown for the islands and the wetting layers, respectively.

In summary, temperature- and power-dependent PL measurements were carried out on the multilayer structure of Ge islands grown on a Si(001) substrate by gas-source MBE. Different power-dependent behaviors of the PL peak position were observed for the wetting layer and the islands. Accordingly, type-II and type-I band alignments are proposed for the islands and the wetting layers, respectively. In addition, the PL intensity from the islands increased significantly as the temperature increased from 8 to 20 K, while the PL intensity of the wetting layer decreased rapidly. The transfer of photon-induced carriers from wetting layers to the islands and the region near to the islands is evidenced.

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