Transition from direct to indirect band structure induced by the AlSb layer inserted in the GaSb/AlSb quantum well

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A 6.5-nm coupled double GaSb/AlSb quantum well separated by 1, 2, 3 or 4 monolayers AlSb has been investigated by photoluminescence spectroscopy at a temperature of 2 K. When the AlSb layer thickness is more than 1 monolayer (ML), this system changes from direct to indirect energy-band structure, which is well described by a model based on a finite potential well and transmission probability.
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GaSb/AlSb quantum wells are of great interest because in this material system a number of new quantization induced phenomena have been observed, which are absent in other systems.[1–6] GaSb is only barely a direct-gap semiconductor. The L valley is only about 85 meV above the Γ valley. The effective mass of the electrons in the L valley is about 10 times higher than that in the Γ valley. When the well width is less than about 4 nm, quantum confinement will push the Γ valley above the L valley and the system changes from direct to indirect band structure.[4] In the field of transport properties and tunneling, the effective masses of carriers play an important role. Recently, some reports about GaSb/AlSb double-barrier heterostructures have indicated that the anomalous I-V curve is related to the great difference of electron effective mass in the Γ and L valley.[7–9]

In contrast to previous reports focusing on the size-induced transition from direct to indirect band structure, this work, to our knowledge for the first time, shows that the insertion of a AlSb layer in the center of a single quantum well can also induce this band-structure change.

Investigation of the transition from direct to indirect band structure is a very interesting topic in this GaSb/AlSb system. Based on this idea, this work designed a set of samples that are a GaSb/AlSb single quantum well separated by inserting 1, 2, 3 or 4 monolayer AlSb in the center of the well. A suitable single quantum well structure should have a width L_z above the Γ/L crossover (i.e., well width >4 nm) and $\frac{1}{2}L_z$ should be below the Γ/L crossover. The thickness of the AlSb layer is increased step by step until the single quantum well is completely divided into two single quantum wells.

The quantum well structures were grown on (001) GaAs substrates. The substrates were cleaned, etched, mounted and heat cleaned as for homoepitaxial molecular-beam-epitaxy growth of GaAs. An AlSb layer is chosen as an intermediate buffer because there exists an extremely wide window for good epitaxial growth of AlSb on GaAs. In a first step, a 300-nm GaAs buffer layer was grown before a 200-nm AlSb buffer, because the GaAs buffer layer can provide a good surface for AlSb nucleation. Despite the large lattice mismatch between AlSb and GaAs (~7%), smooth epitaxy of AlSb results after 200 nm, followed by a 6.5-nm single GaSb quantum well with an AlSb layer inserted in the center of the well and a 40-nm AlSb barrier. Finally, the structure was capped with a 10-nm GaSb layer in order to protect it from oxidation. In order to obtain a mirrorlike surface, the ratio of [Sb]/[Ga] should be about 10. The growth temperature of AlSb nucleation layer and GaSb well are 610 and 585 °C, respectively. The structures of these samples are shown in Fig. 1, i.e., a single quantum well with n monolayers AlSb (n=1, 2, 3, 4; 1 monolayer is approximately 3.1 Å) inserted in the middle.

Photoluminescence (PL) measurements were performed at a temperature of 2 K. The samples were excited by the 647-nm line of a cw Kr ion laser. As to the excitation power, 7.5 mW was used to excite the sample without an AlSb layer and the sample with a 1 ML AlSb layer, 110 mW was used to excite the samples with a 2–4 ML AlSb layer because the intensities of these samples decrease greatly. The photoluminescence was dispersed by a 0.25-m monochromator and detected by a liquid-nitrogen-cooled germanium detector and a lock-in amplifier.

The PL spectra of these samples are shown in Fig. 2. For the single quantum well without an AlSb layer, the situation is very simple. Since this thickness is larger than required for the Γ/L crossover, the luminescence is due to a direct transition. Therefore, the PL spectrum shows only one peak that corresponds to the transition between the Γ electron in the $n=1$ conduction subband and heavy hole in the $n=1$ valence subband. Using the finite potential-well model, the transition energy is calculated to be approximately 0.936 eV,

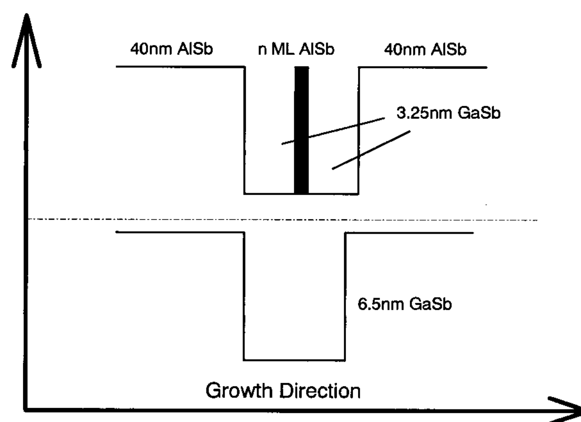

FIG. 1. The structures of coupled double quantum wells (n=1, 2, 3, 4).

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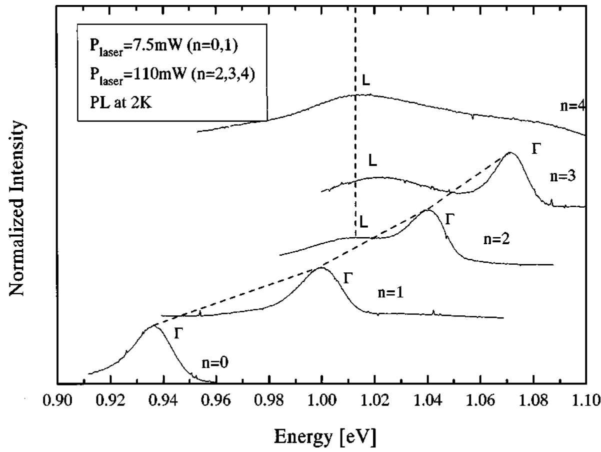

FIG. 2. Photoluminescence spectra of coupled double quantum wells separated by the AlSb layers of different thicknesses at a temperature of 2 K. When the AlSb layer is less than 2 ML, the excitation power is 7.5 mW. When the AlSb layer is more than 1 ML, the excitation power is 110 mW. The dashed line is a guide to the eye.

which agrees with the spectral position of the PL line of 0.9367 eV. However, when the single quantum well is separated by inserting n monolayers AlSb layer in its center, the exciton wave functions and the quantization effects of Γ and L electrons are modified differently due to the great difference in their effective masses. In the photoluminescence spectra shown in Fig. 2, for less than 2 ML AlSb, only one peak appears. However, from the case of 2 ML AlSb, there appears another weak peak the position of which is almost independent of the thickness of the AlSb layer. The intensity of this peak increases with increasing thickness of the AlSb layer. When the AlSb layer reaches 4 ML, the strong peak at the high-energy position disappears.

The peaks at the high-energy position side are from the transition in the Γ valley in each spectrum while the peaks at the low-energy position are just from the transition in the L valley. In order to explain the experimental results, first, the electron wave functions in the L and Γ valleys are calculated, which are shown in Fig. 3. The effective masses and potential for the Γ and L electrons were taken from Ref. 10. A finite potential well model was used in this calculation. Figure 3 gives the square of the electron wave functions in the L and Γ valleys. In the case of the electron wave functions in the L valley, one can find that the coupling between two quantum wells with $\frac{1}{2}L_z$ width decreases with increasing AlSb thickness. In fact, from the case of 2 ML AlSb, the coupling has already disappeared, which is clearly indicated in Fig. 3. It means that a 2 ML AlSb separates a L_z-wide single quantum well into two $\frac{1}{2}L_z$-wide single quantum wells without any coupling for the electrons in the L valley. But in the case of the electron wave functions in the Γ valley shown in Fig. 3, the coupling between two quantum wells still works up to 4 ML AlSb. This results are attributed to the transmission probability which is given by[11]

$$T \propto \exp\left[\frac{-2a(2m_0^*)^{1/2}(V-E)}{\hbar}\right].$$

Here, a is the thickness of the barrier, m_0^* is the effective mass of the carriers, V is the potential of the barrier, E is the energy of carrier, and $\hbar$ is Planck's constant.

From this equation, it can be seen that the transmission probability decreases exponentially with the increase of the effective mass and thickness of the barrier. It is well known that the effective mass of the electron in the L valley is 10 times higher than that of the electron in the Γ valley. Therefore, the transmission probability of the electrons in the L valley decreases much more quickly than that of the electrons in the Γ valley with increasing AlSb thickness.

This work also gives the calculations of the transition energies that can compare with the PL results. The calculation results are shown in Fig. 4.

The dashed lines correspond to the calculated transition energies in the L and Γ valley described in detail in Fig. 4. The circle point (○) and the solid square point (■) correspond to the transition energies in the Γ valley and L valley

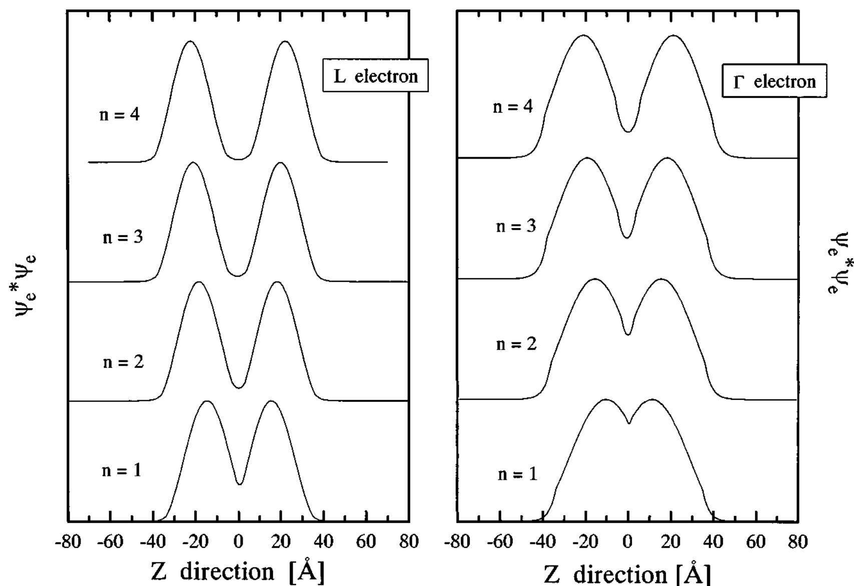

FIG. 3. The square of electron wave functions in the L and Γ valley vs thickness of AlSb.

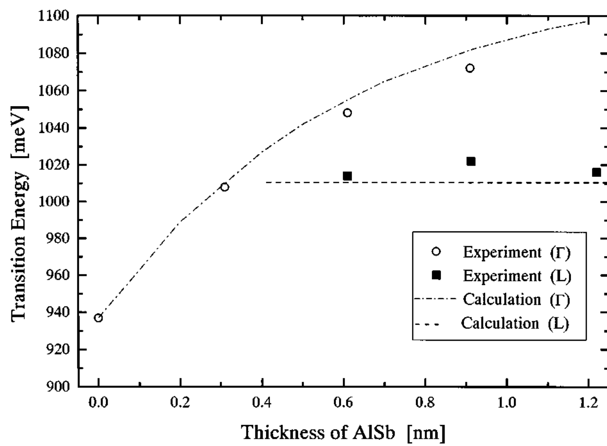

FIG. 4. Thickness of AlSb layer dependence of the transition energies observed in the photoluminescence spectra. The curves represent the calculated transition energy of the Γ and L electrons.

from the PL spectra in Fig. 2, respectively. From above discussion, it is clear that this structures from the case of 2 ML AlSb are just two single quantum wells for the electrons in the L valley. Therefore, the calculations for the transition in the L valley is just transition energy of 3.25-nm-wide single quantum wells. It should not depend on the AlSb thickness. The transition energy of a 3.25-nm-wide GaSb well in the L valley (from $n=1$ conduction subband→heavy hole in the $n=1$ valence subband) is calculated to be 1.01 eV. From Fig. 4, it can be found that the position of the weak peaks is almost at 1.01 eV. From the calculation, one can also find that from the case of 2 ML AlSb the transition energies is smaller than that of the transitions in the Γ valley. This means that the band structures from the case of 2 ML AlSb changes from direct to indirect.

The intensities of the PL also prove this above discussion. For the case of zero ML and 1 ML AlSb, the intensities of PL are very large, we used the excitation power of 7.5 mW. From the case of 2 ML AlSb, the intensities of the PL decrease very quickly. The used excitation power is increased to 110 mW. Since the indirect transitions are associated with the participation of phonons, the intensities should decrease greatly. From above discussion, one can definitely conclude that 2 ML or more AlSb inserted in the middle of the 6.5-nm-wide quantum well can induce the transition from direct band structure to indirect band structure.

In conclusion, we have investigated the photoluminescence of coupled double quantum well separated by AlSb layer. When the AlSb layer thickness is above 1 ML, this system changes from direct to indirect band structure. The calculations based on a simple model are in good agreement with the experimental results.

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