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Effect of Barrier Configuration and Interface Quality on Structural and Electronic Properties of MBE Grown $GaAs/Al_xGa_{1-x}As$, $GaSb/Al_xGa_{1-x}Sb$, and $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ Superlattices

Klaus Ploog

Max-Planck-Institut für Festkörperforschung

D-7000 Stuttgart-80, FR-Germany

The challenge for the design and growth of quantum wells and superlattices made of III-V semiconductors is to minimize scattering from impurities, alloy clusters or interface irregularities so that the confined carriers can move freely along the interfaces. We present a few examples for the influence of interface quality and barrier configuration on the structural as well as electrical and optical properties of III-V semiconductor quantum wells and superlattices grown by molecular beam epitaxy (MBE).

1. Introduction

The fabrication of ultrathin semiconductor layers and multiple layers with abrupt junctions and precise dopant control plays an important role for the development of new photonic and electronic devices. The technique of molecular beam epitaxy (MBE) provides atomic abruptness and smoothness between layers of different lattice-matched and lattice-mismatched III-V semiconductors at their interfaces or heterojunctions. The heterointerfaces between epitaxial layers of different composition ($GaAs/Al_xGa_{1-x}As$, $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$, $GaSb/Al_xGa_{1-x}Sb$, etc.) are used to confine electrons or holes to two-dimensional (2D) motion. The challenge for the design and growth of materials is to minimize scattering from impurities, alloy clusters or interface irregularities so that the carriers can move freely along the interfaces. In this paper we present a few selected examples for the influence of barrier configuration and interface quality on the structural and electronic properties of quantum wells (QW) and superlattices (SL) made of III-V semiconductors. The material systems GaAs/AlAs, $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$ and GaSb/AlSb are attractive for application in advanced photonic devices, as they cover the 0.6 - 2.0 µm wavelength range in emission and absorption, and in high-speed devices because of the formation of high-mobility 2D electron and hole systems.

2. Results and Discussion

2.1 Interface roughness (or disorder)

Since MBE growth occurs predominantly in a 2D layer-by-layer growth mode, the compositional changes at heterointerfaces of closely lattice-matched materials should occur over no more than one monolayer. However, for the widely used $GaAs/Al_xGa_{1-x}As$

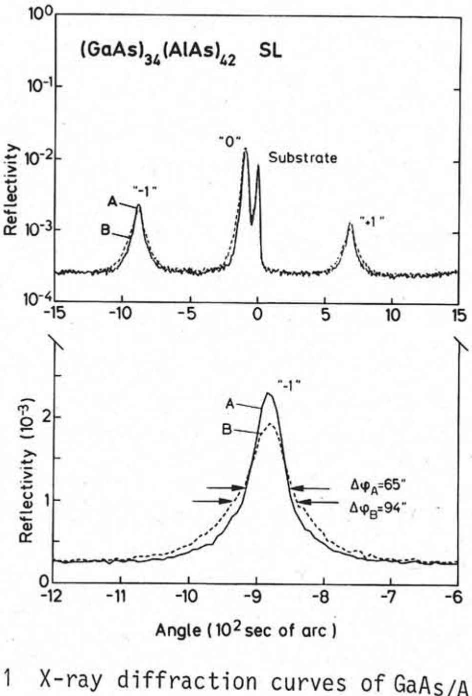

Fig. 1 X-ray diffraction curves of GaAs/AlAs superlattices grown with (A) and without (B) growth interruption at the heterointerfaces, recorded with $CuK\alpha_1$ radiation in the vicinity of the quasi-forbidden (002) reflection.

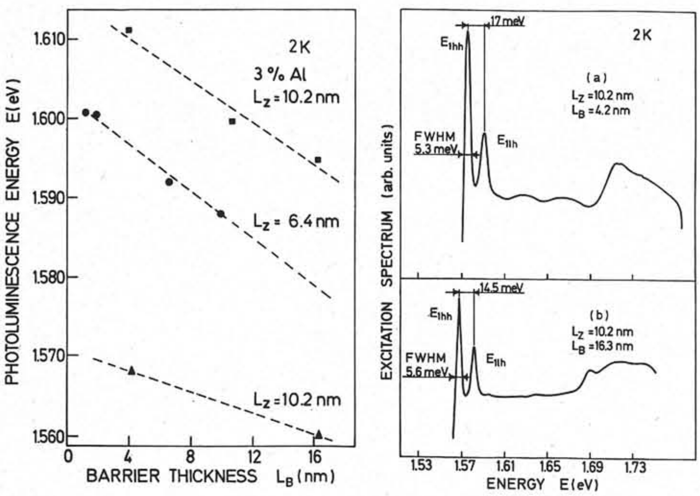

Fig. 2 Variation of luminescence energy (left) and splitting between E_{1h} and E_{1l} free-exciton resonances (right) as a function of barrier thickness in GaAs/AlAs SL.

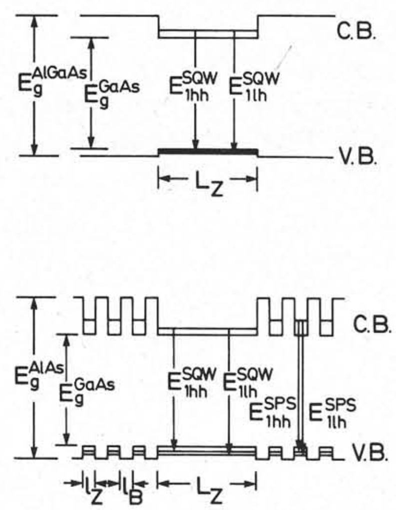

Fig. 3 Real-space energy band diagram of GaAs QW confined by ternary $Al_xGa_{1-x}As$ alloy (top) or by all-binary GaAs/AlAs SPS (bottom).

heterojunction it is well established that the sequence of layer growth is critical for compositional gradients and crystal perfection, which in turn strongly affect the excitonic and the transport properties of QW. While the GaAs/$Al_xGa_{1-x}As$ heterointerface is abrupt to within one monolayer when the ternary alloy is grown on the binary compound, this is not the case for the inverse growth sequence under typical MBE growth conditions [1]. This phenomenon is probably caused by the difference in the relative surface diffusion lengths of Ga and Al on (100) surfaces [2]. Various attempts have been made to minimize the interface roughness (or disorder) by modifying the MBE growth conditions. The most successful modification is the method of growth interruption at each interface, which allows the small terraces between monolayer steps on the $Al_xGa_{1-x}As$ surface to relax into larger terraces via diffusion of the surface atoms, and thus reduces the step density. The time of closing both the Al and the Ga shutter (while the As shutter is left open) depends on the actual growth conditions and values ranging from a few seconds to several minutes have been reported.

High-angle X-ray diffraction is a powerful nondestructive technique for investigation of interface disorder effects in superlattices, if a dynamical analysis of the diffraction curves is performed [3]. From the halfwidth and intensity of the satellite peaks located symmetrically around the Bragg reflections detailed information about thickness fluctuations of the constituent layers, inhomogeneity of composition, and interface quality can be extracted. The existence of interface disorder manifests itself in an increase of the halfwidth and a decrease of the intensity of the satellite peaks, as shown in Fig. 1 for the GaAs/AlAs SL sample B. Sample A was grown with growth interruption at each interface, while sample B was grown continuously. The monolayer roughness of the growth surface during continuous growth leads to a disorder and thus broadening of the interface. During X-ray diffraction this broadening manifests itself as a random variation of the superlattice period of about one lattice constant (~ 5.6 Å) for sample B.

2.2 Effect of Barrier Thickness on Luminescence

When the barrier thickness L_B in GaAs/Al_xGa_{1-x}As SL is reduced to below 3 nm, the wavefunctions of the GaAs wells couple through the barriers and subbands of finite width parallel to the layer plane are formed. At this transition from a multi QW heterostructure with isolated GaAs wells to a real Esaki-Tsu SL the luminescence peak energy decreases for a constant well width L_z due to the broadening of the subbands. We have recently found, however, that even for isolated GaAs wells with thick barriers in GaAs/AlAs SL the barrier thickness has an unexpected influence on the excitonic transitions [4]. In Fig.2 we show that for constant GaAs well widths of L_z = 10.2 nm and L_z = 6.4 nm

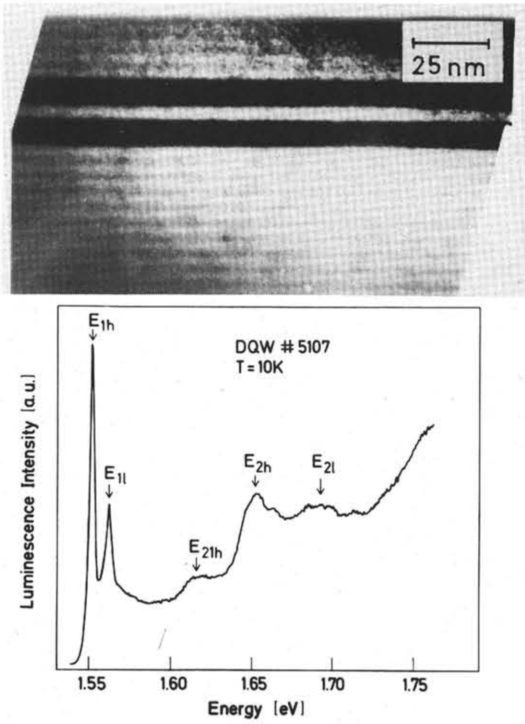

Fig. 4 (110) cross-sectional TEM (top) and PLE spectrum (bottom) of a 9-nm GaAs double QW structure confined by $Al_{0.24}Ga_{0.76}As$ SPS due to compositional oscillations induced by substrate rotation.

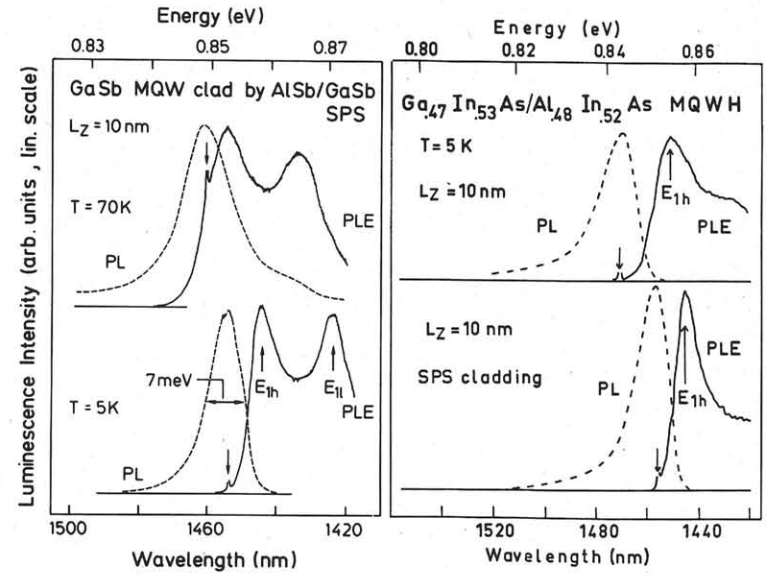

Fig. 5 Low-temperature PL and PLE spectra of GaSb QW confined by SPS (left) and of $Ga_{0.47}In_{0.53}As$ confined by ternary $Al_{0.48}In_{0.52}As$ and by $Ga_{0.47}In_{0.53}As/Al_{0.48}In_{0.53}As$ SPS (right).

the excitonic peaks shift to higher energies and the splitting between heavy- (E_{1h}) and light-hole (E_{1l}) free excitons becomes larger when the AlAs barrier thickness is reduced from L_B = 16 to L_B = 2 nm. The same high-energy shift exists when 3 mole percent Al is added to the well. This phenomenon is in contrast to the expectation from a simple coupling between adjacent wells, and a conclusive explanation has not yet been found. For interpretation we have to take into account the complex band structure of GaAs QW arising from (i) the valence band mixing, (ii) the non-parabolicity of the conduction band, and (iii) the indirect nature of the barrier material. For practical application it is important that our results demonstrate the inadequacy of luminescence spectroscopy to determine the well widths of superlattice accurately. For this purpose additional techniques like double-crystal X-ray diffraction are required.

2.3 Short-Period Superlattice Barriers

The concept of short-period superlattice (SPS) barriers was originally developed to replace the ternary alloy $Al_xGa_{1-x}As$ by all-binary GaAs/AlAs SL [5] because (i) $Al_xGa_{1-x}As$ is an indirect semiconductor for x > 0.4, (ii) deep donors exist in n-doped $Al_xGa_{1-x}As$ for x > 0.2, and (iii) the growth sequence $Al_xGa_{1-x}As$/GaAs exhibits considerable disorder at the interface. In Fig. 3 we show schematically the energy band edges of a GaAs QW confined either by homogeneous ternary $Al_xGa_{1-x}As$ barriers or by GaAs/AlAs SPS barriers. The effective barrier height for carrier confinement in the QW is adjusted by appropriate choice of the layer thickness of the lower-gap material in the SPS.

Several years before we studied the improvement of the optical properties of GaAs, GaSb, and $Ga_{0.47}In_{0.53}As$ QW by using SPS barriers systematically, we had already unintentionally produced periodic compositional oscillations in the growth direction of $Al_xGa_{1-x}As$ barriers, as shown in Fig. 4, which were related to the substrate rotation. The regular fringes observed in the dark-field TEM through the cross-section of a GaAs double QW structure were caused by compositional oscillations with a period of 5 nm, due to variations of the Ga and Al flux profiles over the substrate area. The observed period was consistent with the growth rate of 1.2 µm/hr and the substrate rotation frequency of 4 rpm. Although not intentionally introduced and often undesired, in that particular case the periodic variation of the $Al_xGa_{1-x}As$ alloy composition normal to the layers resulted in highly improved

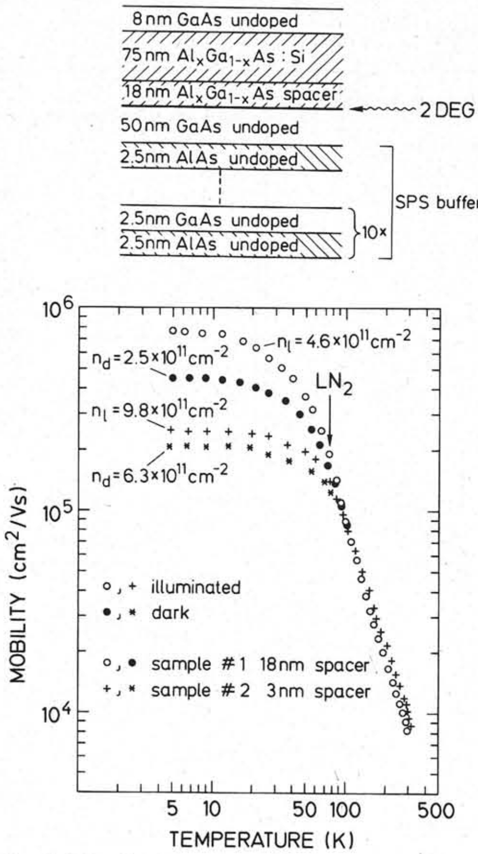

Fig. 6 Hall electron mobilities versus temperature obtained from two selectively doped GaAs/$Al_xGa_{1-x}As$ heterostructures with different spacer widths whose configuration is schematically shown at the top.

luminescence properties of GaAs QW as shown by the photoluminescence excitation (PLE) spectrum in Fig. 4. In addition to the parity-allowed n = 1 and n = 2 electron heavy- and light-hole exciton resonances, also a forbidden transition (E_{21h}) was observed at 1.62 eV. The very sharp exciton resonances and the large intensity ratio of the E_{1h} and E_{11} transition (about 3 to 1) indicate the excellent quality of this GaAs QW, in particular the smoothness of the heterointerfaces that were grown four years ago without any growth interruption. We assume that the observed improvement of the optical properties of SPS confined QW is due (i) to a removal of substrate defects by the SPS layers, (ii) to an amelioration of the interface between QW and barrier, and (iii) to a modification of the dynamics of injected carriers in the SPS barrier.

The application of SPS barriers has an even more dramatic effect on the improvement of excitonic recombinations processes in GaSb and $Ga_{0.47}In_{0.53}As$ QW [6, 7]. In Fig. 5 we display the results of photoluminescence (PL) and PLE measurements. In GaSb QW the effect of strain and the formation of defect centers at the interface, due to the considerable lattice mismatch of $\Delta a/a_0$ = 0.65% between GaSb and AlSb, is significantly reduced by all-binary GaSb/AlSb SPS confinement layers. As a result the luminescence of SPS confined GaSb QW is dominated by free-exciton emission in the temperature range 4 - 200 K. The small value of 7.5 meV at 5K for the Stokes shift between PL and PLE heavy-hole excitonic peak indicates the absence of impurity related trapping of excitons in the GaSb QW. The application of all-ternary $Ga_{0.47}In_{0.53}As$ /$Al_{0.48}In_{0.52}As$ SPS to confine $Ga_{0.47}In_{0.53}As$ QW resulted in the first experimental evidence for intrinsic free-exciton recombination in this material system. The narrow linewidth of 3.1 meV for the E_{1h} exciton peak in the PLE spectrum and the small Stokes shift of 6.5 meV between PL and PLE exciton peaks manifest the excellent quality of the SPS confined $Ga_{0.47}In_{0.53}As$ QW lattice-matched to InP substrates which were grown without any growth interruption at the heterointerfaces.

A final distinct example for the removal of substrate defects by SPS buffer layers and for the improvement of the interface between QW and SPS barrier is given by a modified selectively doped GaAs/$Al_xGa_{1-x}As$ heterostructure with high-mobility 2D electron gas (2DEG) [8], whose layer sequence is schematically shown in Fig. 6. The 10-period GaAs/AlAs SPS prevents propagation of dislocations from the substrate so that the thickness of the "active" GaAs layer containing the 2DEG can be reduced to 50 nm. The results of Hall effect measurements (Fig. 6) demonstrate the excellent mobilities of the 2DEG obtained for two samples with different spacer widths. The SPS-confined narrow "active" GaAs layer of the heterostructure is of distinct importance for transistor operation, because the electrons cannot escape too far from the 2D channel during pinchoff. This implies a higher transconductance for the HEMT. Finally, the growth time of the complete heterostructure is reduced to less than 15 min. An additional 15 min for wafer exchange and heat and cool time makes a total of 30 min throughput time per high-quality heterostructure wafer grown by MBE.

3 Conclusion

The heterointerfaces between epitaxial layers of different III-V semiconductors are used to confine electrons and holes to 2D motion. We have presented a few examples for the effect of barrier configuration and interface quality on the structural and electronic properties of quantum wells and superlattices formed by the material systems GaAs/AlAs, $Ga_xIn_{1-x}As/Al_xIn_{1-x}As$, and GaSb/AlSb. A careful analysis of the X-ray diffraction data obtained from GaAs/AlAs superlattices revealed that the interface disorder can be minimized by growth interruption at each heterointerface. In contrast to previous assumptions for uncoupled GaAs quantum wells, the excitonic peaks shift to higher energies when the AlAs barrier thickness is reduced from 16 to 2 nm, due to the complex band structure of this QW system. The introduction of short-period superlattices as barriers resulted in a substantial improvement of the optical and electrical properties of GaAs, GaSb, and $Ga_{0.47}In_{0.53}As$ quantum wells and heterostructures.

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