Measurement of the direct energy gap of $Al_{0.5}In_{0.5}P$: Implications for the band discontinuity at $Ga_{1-x}In_xP/Al_yIn_{1-y}P$ heterojunctions

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In a recent paper [Phys. Rev. B **48**, 18 031 (1993)], Patel and co-workers described hydrostatic-pressure-dependent photoluminescence measurements performed on $Ga_{0.47}In_{0.53}P/Al_{0.5}In_{0.5}P$ multiple quantum wells. They determined directly a valence-band offset of 0.24±0.05 eV from the energy difference between the indirect transition in the barrier and the transition from X states in the barrier to hh1 valence-band states in the quantum well, when extrapolated to zero pressure. The conduction-band offset was then indirectly determined to be 0.26 eV from the total-band discontinuity of the system, assuming a value of 2.45 eV for the (low temperature) lowest-energy direct gap of $Al_{0.5}In_{0.5}P$. This yields a band-offset ratio, $\Delta E_c:\Delta E_v$, of 52:48. Here, we present evidence that the (5 K) direct gap of the $Al_{0.5}In_{0.5}P$ barrier is ~2.685 eV, which results in a revised band-offset ratio of 67:33, similar to recent values determined for $Ga_{1-x}In_xP/(Al_yGa_{1-y})_{0.5}In_{0.5}P$ heterojunctions.

A recent paper[1] by Patel, Hafich, Robinson, and Menoni describes a determination of the band discontinuities in $Ga_{0.47}In_{0.53}P/Al_{0.50}In_{0.50}P$ multiple quantum wells, from low-temperature photoluminescence (PL) measurements performed at high pressure (up to 4 GPa). This material system shows a type-I band alignment for the direct gap and a type-II alignment for the indirect X minima at ambient pressure. As described in Ref. 1, it is possible, by applying hydrostatic pressure, to induce a transition involving recombination from the barrier X minimum (X_b) to the first confined heavy-hole valence-band state (hh1) in the $Ga_{1-x}In_xP$. By extrapolating the energy of this transition to 0 GPa, and subtracting it from the energy of the barrier PL, the valence-band offset can be directly determined. The authors of Ref. 1, report the use of this technique to obtain a valence-band discontinuity of 0.24±0.05 eV for this system. Determination of the conduction-band discontinuity, however, requires a knowledge of the lowest-energy direct gap of the barrier material. In Ref. 1 a literature value[2] of 2.45 eV is used for the low-temperature Γ gap of the barrier. This results in a band-offset ratio, $\Delta E_c:\Delta E_v$, of 52:48. It is the purpose of this paper to present evidence that the direct gap of the $Al_{0.5}In_{0.5}P$ barrier is ~2.685 eV, which when combined with the observations in Ref. 1 results in a band-offset ratio of 67:33, similar to recent values determined for $Ga_{0.52}In_{0.48}P/(Al_yGa_{1-y})_{0.52}In_{0.48}P$ heterojunctions.[3,4]

Relatively few studies have reported on the lowest-energy direct gap E_Γ for $Al_{0.5}In_{0.5}P$. These[2,5–7] have typically been performed at room temperature, using techniques including electroreflectance, optical absorption, and cathodoluminescence. The majority of values (at 300 K) are in the range 2.51–2.57 eV, from which low-temperature (5–20 K) values of ~2.6–2.7 eV are anticipated. Reference 1 uses a low-temperature value of 2.45 eV, estimated from the 300-K measurements of Ref. 2, which is significantly lower than the more recent values.[7] In the following, we describe photoluminescence excitation spectroscopy (PLE) measurements performed on lattice-matched $Al_{0.5}In_{0.5}P$-on-GaAs samples, which allows E_Γ at 5 K for $Al_{0.5}In_{0.5}P$ to be determined directly.

Growth was performed by gas-source molecular-beam epitaxy simultaneously on quarter wafers of GaAs offcut by 0°, 7°, 10°, and 15° from (100) to nearest (111)A. In agreement with previous reports,[7] we had found the higher offcut angle substrates to suppress the effects of atomic ordering on the group-III sublattice for growth of $Ga_{0.5}In_{0.5}P$. No effect of substrate orientation on the measured PL or PLE spectra was observed, however, for $Al_{0.5}In_{0.5}P$, grown under similar conditions. The results reported here were all taken on the on-orientation (100) sample. $Al_{0.5}In_{0.5}P$, of thickness 2 μm, was deposited following a 1-μm GaAs buffer layer. A 100-Å $Ga_{0.5}In_{0.5}P$ protective cap completed the structure. Double crystal x-ray-diffraction rocking curves indicated a composition of $Al_{0.511}In_{0.489}P$ for the epilayer, with a mismatch from the substrate of only 192 ppm. PLE spectra were obtained at 5 K, with the sample mounted in a helium flow cryostat. The optical excitation source was a tungsten-halogen lamp/0.22-m monochromator combination; the

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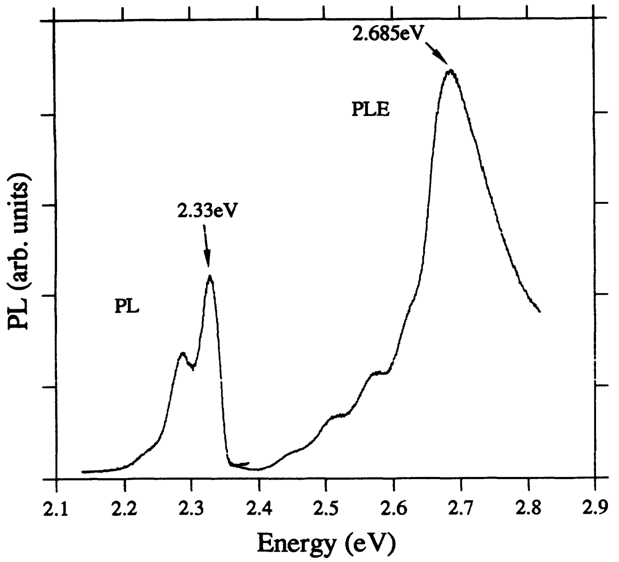

FIG. 1. 5-K PL and PLE spectra of bulk $Al_{0.5}In_{0.5}P$ epilayer.

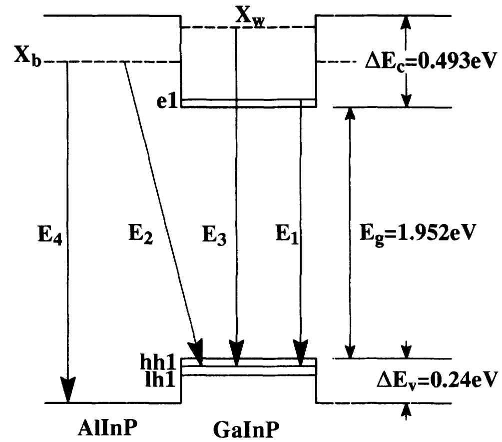

FIG. 2. Band-structure schematic (5–20 K) for a $Ga_{0.47}In_{0.53}P/Al_{0.5}In_{0.5}P$ quantum well using the valence-band discontinuity of Ref. 1, and the lowest-energy direct gap determined in the present work. Labeling of the transitions is as described in the text.

detection system consisted of a 0.5-m spectrometer, cooled GaAs photomultiplier, and photon-counting electronics. The overall spectral resolution of the measurements was ~ 3 meV.

Figure 1 shows typical PL and PLE spectra obtained. The PL peak is at 2.336 eV, which compares closely with the value obtained in Ref. 1 (2.35 ± 0.01 eV). The main peak in the PLE, ascribed to the E_Γ transition, is observed at 2.685 eV. We have also obtained very similar data from $Al_{0.5}In_{0.5}P$ samples grown by solid source molecular-beam epitaxy. The value for E_Γ is slightly (~ 20 meV) on the high side of the range anticipated from extrapolation of the room-temperature values listed above. We believe, however, that the result is supported by the high quality of our sample (as evidenced by the x-ray diffraction and optical data using lamp illumination) and the directness of the measurement technique. Weak fringes evident in the rising edge of the PLE between 2.4 and 2.65 eV are due to Fabry-Perot interference between the epilayer surface and $Al_{0.5}In_{0.5}P/GaAs$ interface, but have no significant effects on the measurements.

In the following discussion, we hold to the labeling and identification of the transitions given in Ref. 1. E_1 is identified as recombination in the well from the $e1$ lowest confined conduction-band state to the hh1 heavy-hole valence-band state, E_2 as involving the X_b states in the barrier and the hh1 valence-band state in the well, E_3 is assigned to recombination from the well X_w minimum to well hh1, and E_4 to recombination in the barrier from X_b to the barrier valence band.

In Fig. 2, we show a schematic diagram of the (low temperature) band alignment of the $Ga_{0.47}In_{0.53}P/Al_{0.5}In_{0.5}P$ quantum wells, which we propose, on the basis of our determination of the $Al_{0.5}In_{0.5}P$ Γ gap, be substituted for Fig. 7 in Ref 1. We retain the values for the direct band gap of bulk $Ga_{0.47}In_{0.53}P$ (1.952 eV) and the valence-band offset (0.24 eV) which the authors of Ref. 1 determined directly. Substituting our value for the barrier Γ gap then implies a conduction-band discontinuity of 0.493 eV. This corresponds to a band-offset ratio of 67:33, which is similar to recent determinations for $Ga_{0.5}In_{0.5}P/(Al_yGa_{1-y})_{0.5}In_{0.5}P$ heterojunctions.[3,4] In these reports, the band offsets were determined as an adjustable parameter required to achieve a comprehensive fitting of all optical transitions observed by PLE in quantum wells having a range of well widths.

In conclusion, on the basis of a direct determination of the lowest-energy direct Γ gap of $Al_{0.5}In_{0.5}P$, independently confirmed in our two laboratories, we propose a modification to the band structure for $Ga_{0.53}In_{0.47}P/Al_{0.5}In_{0.5}P$ heterojunctions given in Ref. 1. Substitution of our value gives a band-offset ratio for the system of 67:33, which is similar to recent determinations for $Ga_{0.5}In_{0.5}P/(Al_yGa_{1-y})_{0.5}In_{0.5}P$ quantum wells obtained by a comprehensive fitting of transitions observed by low-temperature PLE.

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