Optical studies of GaAs quantum wells strained to GaP

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Quantum wells of GaAs lattice matched to GaP have been studied by photoluminescence and electroreflectance. The quantum well thickness was varied between 1 and 6 monolayers in steps of 1 monolayer. Electron-hole transitions have been observed involving states both in the X band and in the \( \Gamma \) band, which have been modeled using a k.p. model in conjunction with the envelope function approximation. Overall agreement between theory and experiment is found using an unstrained valence band offset of 0.6 eV. © 1997 American Institute of Physics.

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In strained semiconductor structures the lattice parameter and the band gap are independent variables. This is also true for quaternary alloys and in conjunction with strain, many degrees of freedom are available for the engineer. Strained semiconductor structures are essential in important many degrees of freedom are available for the engineer. Strained semiconductor structures are essential in important

Most of the work has been performed on semiconductors having a direct band gap. Work on strained materials having indirect band gaps such as Si–Ge, AlAs–InAs, and GaP–GaAsP has also been performed. We will report in this letter on the optical properties of GaAs quantum wells (QWs) of strained to GaP, as a natural extension of the work published in Refs. 7 and 8. We have studied electronic transitions related to both the \( X \) minima and to the \( \Gamma \) minimum of the conduction band, using photoluminescence (PL) and electroreflectance (ER), respectively. The transition energies have been modeled using an eight-band k.p. model, in conjunction with the envelope function approximation.

The samples were grown by atomic layer molecular beam epitaxy (ALMBE) on undoped (001) \( \pm 0.5^\circ \)-oriented GaP substrates. Each sample contains three GaAs layers of equal thickness, ranging from 1 to 6 monolayer (ML), separated by sufficiently wide (38 nm) GaP barriers to assure no coupling between adjacent GaAs well layers. The lattice mismatch is 3.6% and the critical thickness for dislocation formation should be of the order of 6 ML, close to the observed value for GaP grown on GaAs. The growth rate was 1 \( \mu \)m/h and the growth temperature was 400 °C. Observed reflection high-energy electron diffraction patterns correspond to a clear two-dimensional growth mode. In all the samples, an initial GaP buffer layer with a thickness of 0.7 \( \mu \)m was grown by molecular beam epitaxy (MBE). The confined phonon frequencies of the samples have been measured by Raman spectroscopy. The experimental frequencies agree very well with theoretical calculations assuming fully strained GaAs layers and a moderate degree of intermixing at the interfaces. The best agreement is obtained assuming an As carry-over at the upper interface (probably induced by strain), with a segregation coefficient of about 0.5.

Figure 1 shows the calculated potential structure of GaAs biaxially strained to GaP. The calculation is based on deformation potential theory, using six bands for the valence band and treating the \( X \) band and the \( \Gamma \) band separately. The parameters for the calculation are taken from Ref. 14, with the exception of the hydrostatic deformation potential of the band gap \( (a_p) \) of GaAs, which was taken to be \( -8.5 \) eV in order to fit the data in Ref. 15. We assume that the valence band offset does not depend on hydrostatic strain. The few experiments that have addressed this question agree with this assumption, but more work is needed for general conclusions to be drawn about this important parameter. An unstrained valence band offset of 0.6 eV (giving a strained valence band offset of 0.7 eV) was used in the figure, which gives the best fit to the experiment, as will be shown later. From now on we will use the abbreviation VBO for the unstrained valence band offset. It can be seen that the GaAs layer is indirect in the \( k \) space, due to the strain. The lowest conduction band minima are the \( X_{xy} \) minima in which the \( k \) vector is in the layer plane. The \( X \) conduction band minimum with the \( k \) vector is in the growth direction and appears at higher energies. For a VBO of 0.6 eV the discon-

![FIG. 1. A diagram of the band-edges at \( k=0 \) for the heavy hole and the light hole in the valence band, as well as the \( \Gamma \) minimum and the \( X \) minima of the conduction band for GaAs strained to GaP. The \( X \) minima in GaAs are split into \( X_{xx} \) and \( X_{yy} \), where the subscript indicates the direction of the \( k \) vector and \( z \) is the growth direction. An unstrained valence band offset of 0.6 eV was used for this calculation.](image-url)
The energies of the phonons most closely correspond to 

\[ \text{TA}^5 \] and \[ \text{LA}^5 \] phonon energies in GaP. Phonon-assisted transitions involving \[ \text{LA}^4 \] and \[ \text{TA}^4 \] phonons (instead of the more commonly occurring LO phonons) have previously been observed in indirect GaAsP, both bulk,\textsuperscript{17} as well as strained to GaP.\textsuperscript{8} The relative intensity of the no-phonon line decreases with decreasing thickness of the layers, becoming difficult to resolve for the thinnest QWs. This may be related to the increasing separation between \( \Gamma \) states and \( X \) states for narrower QWs. If the \( \Gamma \) states are closed to the \( X \) states by an in-mixing of the \( \Gamma \) states into the \( X \) states, due to e.g., interface roughness, will give a significant no-phonon transition.\textsuperscript{8} The total emission intensity increases almost linearly with increasing excitation power density and the emission intensity decreases with increasing quantum well thickness. We speculate that the influence of interface roughness is larger for smaller QWs which will increase the transition probabilities.

At the low energy side of the peak there is a broad tail. Photoluminescence spectra taken at higher temperatures (typically 30 K) show only the broad emission. For the 5 ML QW the relative intensities of the narrow peaks are small compared to that of the broad emission and for the 6 ML QW no narrow peaks are observed. This broad emission is attributed to a defect in the strained layer. No emission from the bulk GaP is seen, indicating more efficient trapping of the carriers by the QWs than by defects in the GaP.

At the high energy side of the peak there is a broad tail. Photoluminescence spectra taken at higher temperatures (typically 30 K) show only the broad emission. For the 5 ML QW the relative intensities of the narrow peaks are small compared to that of the broad emission and for the 6 ML QW no narrow peaks are observed. This broad emission is attributed to a defect in the strained layer. No emission from the bulk GaP is seen, indicating more efficient trapping of the carriers by the QWs than by defects in the GaP.
changing $E_v$. A VBO of 0.7 eV gives the splitting of the $X$ band, of about 0.05 eV. The actual thickness of the layers may also be somewhat different from the nominal thickness. Such an effect would affect the thinner QWs the most. We would like to remark that the observation of both $X$- and $\Gamma$-related transitions gives a more reliable value of the VBO than that based on only one of these sets of transitions. The obtained value of the VBO is in reasonable agreement with calculations of the VBO\textsuperscript{18} as well as with experiments based on emission from transition metal impurities in GaAs\textsubscript{P}.$^{19}$ which give a VBO of 0.5 eV and 0.4–0.5 eV, respectively.

In conclusion, we have studied both the $\Gamma$ band and the $X$ band related transitions of GaAs strained to GaP. The thicknesses of the GaAs QWs have been varied in steps of 1 ML between 1 and 6 ML. Using this rather complete experimental information in conjunction with theoretical modeling, we determine an unstrained valence band offset of about 0.6 eV, giving a strained valence band offset of about 0.7 eV.

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$^{12}$P. Castrillo, G. Armelles, J. P. Silvaire, and F. Briones (to be published).


