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Ellipsometric study of GaAs/GaP superlattices

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Ellipsometric measurements were performed to study the \( E_1 \) and \( E_1 + \Delta_1 \) transitions on a set of GaAs/GaP strained-layer superlattices. The experimental results show the existence of small quantum confinement effects.

In the recent years the interest in strained-layer systems has grown considerably. This increase is due to the possibility of using this system as, for example, buffer layers for growing GaAs on Si or as new materials for heterostructure devices. One particular case of interest is the GaAs/GaP superlattices. This system is similar to GaAs/AlAs (both AlAs and GaP are indirect gap materials). The principal difference between both systems is the strain present in the former case because of the lattice mismatch between GaAs and GaP. If the total thickness of the constituent materials is below a certain critical value, the strain is accommodated by elastic deformations. Such deformation modifies the band structure of the superlattice materials and therefore the optical properties of the superlattice. In this letter we present for the first time an ellipsometric study of a set of strained-layer GaAs/GaP superlattices grown by atomic layer molecular beam epitaxy (ALMBE). The results of the above-band-gap transitions are compared with those of the band gap obtained by photoreflectance. In other systems, such as the lattice-matched GaAs/AlAs or strained systems, it has been shown that these transitions far above the band gap show less quantum confinement than near-band-gap transitions. These results are also present in our superlattices.

A set of strained-layer superlattices GaAs\(_m\)GaP\(_m\) with \( m = 2, 3, 4 \) monolayers was grown on 001 GaAs substrates by ALMBE. The period was confirmed by x-ray diffraction measurements. These samples were optically characterized by spectroscopic ellipsometry at room temperature. From these measurements we determine the pseudodielectric function for each sample. The spectra were taken in the energy range of 1.5–3.5 eV. The pseudodielectric function was obtained assuming a two-phase model \(^6\) (ambient superlattice) and neglecting the presence of an overlayer of oxide. The effect of the substrate is negligible in the energy range that we are interested in, because the absorption coefficient of the superlattice is large and, then, the two-phase model is quite reasonable. The pseudodielectric function obtained can be interpreted as an average dielectric function of the superlattice.

In Fig. 1 we show the imaginary part of the pseudodielectric function \( (\varepsilon_r) \) for the three samples studied here. In the low-energy region we observe an oscillation behavior of \( \varepsilon_r \) due to interference effects (the superlattices are transparent in this region). The spectra of the GaAs\(_m\)GaP\(_m\) and GaAs\(_m\)GaP\(_n\) superlattices show a peak and a shoulder at higher energies that we associate to the \( E_1 \) and \( E_1 + \Delta_1 \) transitions, respectively. For the superlattice GaAs\(_m\)GaP\(_n\), both transitions are included in a broad peak. In order to resolve and obtain the energies for both transitions, we calculate numerically the second derivative of the spectra from our ellipsometric data as a function of the photon energy. An appropriate level of smoothing was allowed to remove the noise originated in the differentiation process without distorting the line shape spectra. We fit these spectra with theoretical expressions for the dielectric constant. \(^7\) The best fits were obtained assuming a two-dimensional critical point for both transitions. In Fig. 2 we show the spectra for the second derivative of the imaginary part of the pseudodielectric function together with the theoretical fits for the three samples studied in this work. The values of the energies obtained from the fits are displayed in Table I.

The energies of the transitions \( E_1 \) and \( E_1 + \Delta_1 \) are slightly shifted towards higher energies with respect to those of GaAs bulk material. Moreover, from Raman measurements \(^8\) it has been observed that the GaP layers are expanded in all the samples and for the longest one \((\text{GaAs}_6\text{GaP}_2)\) the GaAs layers are compressed. Therefore, this energy shift of the transitions can be associated to two different effects: quantum confinement and presence of the strain. We will discuss below quantitatively these effects.

![Fig. 1. Imaginary part of the pseudodielectric function \( (\varepsilon_r) \) at room temperature for the samples: (a) GaAs\(_6\)GaP\(_2\), (b) GaAs\(_6\)GaP\(_2\), (c) GaAs\(_6\)GaP\(_2\).](image-url)
To compare these results with the energy values of the band-gap transitions we have made photoreflectance experiments. Such a technique allows us a better determination of the band-gap energy. From the ellipsometric data the energy of such a transition could be obtained from the damping of the oscillations in the pseudodielectric function of the system, but such a value will give a larger error than the value obtained by photoreflectance. We have used the three-point method for obtaining the energy of the transition in the photoreflectance spectra. As an example we present in Fig. 3 two photoreflectance spectra corresponding to the shortest and longest period samples. In Table I we present the energies of the band-gap transitions. As it is observed, the difference between the \( E_0 \) transition of the superlattice and the \( E_0 \) transition of GaAs bulk is higher than the same difference for the \( E_1 \) transitions. This confirms the smaller confinement effects in the higher interband transitions than in the fundamental energy gap.

We have also displayed in Table I the energy values of the \( E_1 \) and \( E_1 + \Delta_1 \) related transitions of alloys with composition equivalent to that of our superlattices. The values for the superlattices are slower than the same values for the alloys. This effect has also been observed in lattice-matched systems and shows the presence of superlattice effects.

Finally, let us compare these results with those of the GaAs/AlAs system. In a sample similar to the longest one (GaAs, GaP\(_4\)), the \( E_1 \) transition is located in GaAs, AlAs, at 3.15 eV. This energy is higher than that of the GaAs/GaP sample (3.05 eV), which indicates that the confinement effects are smaller in GaAs/GaP. This small quantum confinement is certainly due to a reduction of the effective barrier height because of the strain. (The strain reduces the energy difference between the \( E_1 \)-related transitions of GaAs and GaP.) Moreover, in this particular sample (GaAs, GaP\(_4\)) the GaAs layers are under compression (\( \epsilon = 0.7\% \)), then the energy position of the \( E_1 \)-related transitions is affected by two contributions, one due to the strain in the GaAs layers and the other due to the confinement. The contribution due to the strain can be easily calculated: the modification of the energy position of the \( E_1 \)-related transitions in bulk material due to a biaxial strain (\( \epsilon \)) in the plane 001 is equal to

\[
E_1 = E_1 + \Delta_1/2 + \delta E_h - \frac{1}{2} \left[ \Delta_1^2 + \delta E_{001}^2 \right]^{1/2},
\]

\[
E_1 + \Delta_1 = E_1 + \Delta_1/2 + \delta E_h + \frac{1}{2} \left[ \Delta_1^2 + \delta E_{001}^2 \right]^{1/2},
\]

where \( \delta E_h = -\epsilon(2 - 2C_{11}/C_{12})e \) is the hydrostatic component of the stress-induced shift and \( \delta E_{001} = 2b(1 + 2C_{12}/C_{11})e \) is the shear component of the stress-induced shift. With the values of the deformation potentials and elastic constants of Ref. 12 we obtain a value of 45 meV for \( e = 0.7\% \). Then the contribution of the confinement is 95 meV. The confinement can be estimated with a simple model. In such a model the energies of the bulk \( E_1 \)-related transitions are first modified according to Eqs. (1) and (2). The

![FIG. 2. Second derivative of the imaginary part of the pseudodielectric function (dashed line) and theoretical fit (full line) for the samples: (a) GaAs, GaP\(_4\), (b) GaAs, GaP\(_3\), (c) GaAs, GaP\(_2\).](image1)

![FIG. 3. Photoreflectance spectra for the samples: (a) GaAs, GaP\(_3\), (b) GaAs, GaP\(_4\).](image2)

**TABLE I.** Experimental values for \( E_0 \), \( E_1 \), and \( E_1 + \Delta_1 \) transitions. \( x \) is the mean composition of GaP for an equivalent alloy. The values for the \( E_1 \) and \( E_1 + \Delta_1 \) transitions for equivalent alloys were taken from literature.

<table>
<thead>
<tr>
<th>GaAs/GaP</th>
<th>( x ) (% GaP)</th>
<th>( E_0 ) (eV)</th>
<th>( E_1 ) (eV)</th>
<th>( E_1 + \Delta_1 ) (eV)</th>
<th>( E_1 ) (eV)</th>
<th>( E_1 + \Delta_1 ) (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>6/2</td>
<td>0.25</td>
<td>1.58</td>
<td>2.95</td>
<td>3.165</td>
<td>3.09</td>
<td>3.30</td>
</tr>
<tr>
<td>6/3</td>
<td>0.33</td>
<td>1.67</td>
<td>2.96</td>
<td>3.185</td>
<td>3.13</td>
<td>3.34</td>
</tr>
<tr>
<td>6/4</td>
<td>0.40</td>
<td>1.72</td>
<td>3.03</td>
<td>3.25</td>
<td>3.17</td>
<td>3.38</td>
</tr>
</tbody>
</table>

\(^*\text{Reference 10.}\)
confinement is calculated by means of a one-dimensional Kronig–Penney model, where the $L$-point states of the GaAs wells are supposed to be confined by the corresponding $L$ states of the GaP barriers. Assuming a valence-band offset\textsuperscript{13} of 0.4 \text{eV} we obtain the following values: 70, 90, 109 meV for the GaAs$_m$GaP$_n$ ($m = 2, 3, 4$) samples, respectively, whereas the experimental values are 60, 70, 95 meV. Even with this model the agreement is reasonable.

We have obtained by spectroscopic ellipsometry the energies of the $E_i$ and $E_i + \Delta_i$ transitions of a set of GaAs/GaP superlattices. The results show that the confinement effects are very small.


\textsuperscript{6}R. A. A. Azzam and N. M. Bashara, \textit{Ellipsometry and Polarized Light} (North-Holland, Amsterdam, 1977).


