Determination of the deformation potentials of GaAs$_{0.80}$P$_{0.20}$

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Deformation potentials can be determined by measuring the variation of the energy of the electronic transitions with strain. In this work, the hydrostatic and shear potentials of the band-gap electronic transition ($E_0$) and the transitions along the (111) direction ($E_1$) of GaAs$_{1-x}$P$_x$, $x=0.20$, have been determined by electroreflectance characterization of GaAs$_{1-x}$P$_x$ layers with different levels of strain.

The knowledge of the modification of the physical properties of III-V ternary compounds as a function of the composition is a very important subject, mainly due to its great technological importance. However, the variation of some magnitudes with alloy composition still remains unknown.\(^1\)\(^2\) This is the case of the deformation potentials, magnitudes which describe the effect of the strain on the electronic transitions.

In this communication we present experimental results obtained with electroreflectance measurements, which allow for the determination of the deformation potentials of the $E_1$ and $E_0$ transitions for GaAs$_{1-x}$P$_x$ layers with a phosphorus content about 20%. As we will show later in this work, the deformation potentials values can be determined by measuring the variation of the energy of the electronic transitions with strain.

In this work a different level of strain in the GaAs$_{1-x}$P$_x$ ($x=0.20$) layers is obtained by growing layers of constant composition and different thickness on GaAs substrates (lattice mismatch to GaAs, $f_m=-7.2\times10^{-4}$). As lattice mismatch relaxation depends on layer thickness, the residual strain in the GaAs$_{1-x}$P$_x$ layers will change from one layer to another, allowing for the determination of the deformation potentials for GaAs$_{0.80}$P$_{0.20}$ alloys.

The samples studied in this work consisted of a series of different thickness $h$ ($h=60,$ 200, 400 nm) GaAs$_{1-x}$P$_x$ layers of P composition nearly constant (0.2$\leq x \leq 0.24$) grown on semi-insulating GaAs (001) substrates by atomic layer molecular beam epitaxy (ALMBE).\(^3\) Growth substrate temperature $T_s$ was kept at 350 °C and special group V element solid sources with fast acting valves and cracking sections were used. Prior to GaAs$_{1-x}$P$_x$ layer growth, a 100 nm thick GaAs buffer layer was grown by conventional molecular beam epitaxy (MBE) at $T_s=580$ °C.

The experimental procedure which allows for the growth of GaAs$_{1-x}$P$_x$ layers with an accurate control of composition is based on the combination of ALMBE growth and in situ reflectivity difference (RD) characterization technique and has been previously reported.\(^4\) Basically, the experimental procedure developed consists of analyzing the change in the RD signal which experiments on a GaAs (001) surface with different Ga surface coverages when a P$_2$ pulse impinges on it. As the amplitude of the RD signal, under our experimental conditions, can be directly related to the Ga surface coverage,\(^5\) the difference between the RD amplitude before and after a P$_2$ pulse provides the amount of GaP which has been formed, and so far the phosphorus composition of GaAs$_{1-x}$P$_x$ layer.

This procedure allows us to grow GaAs$_{1-x}$P$_x$ layers with the desired phosphorus composition by an appropriate design of the opening time and duration of the pulses of the phosphorus cell.

All samples were characterized by double crystal x-ray diffraction (DCXRD) in the (+) Bragg arrangement for the (004) reflection and in the $\theta + \phi$, $\theta - \phi$ for the (115) reflections. These four rocking curves were taken in the [110] and [110] directions in each sample. From the recorded data and by using a dynamical simulation program, we can obtain both the P composition, always in coincidence with the in situ determined composition, and the residual strain state in the GaAs$_{1-x}$P$_x$ layers.

The energy position of the transitions was obtained by means of electroreflectance measurements. For that purpose a semitransparent gold Schottky barrier was evaporated in the samples and the measurements were made at 80 K. Besides the modulated field, a continuous voltage was applied to the sample. Its magnitude was varied in order to record the spectra in the low field regime.\(^6\) To eliminate the small linear electro-optical (LEO) component present in the spectra of the electronic transition along the (111) direction ($E_1$), the spectra were recorded with the light polarized parallel to the [100] direction.

The effect of a biaxial strain in the (001) plane on the fundamental transition at the $\Gamma$ point of the band structure ($E_0$) can be described by means of two deformation potentials\(^8\) labeled: a (hydrostatic) and b (shear). Such biaxial strain produces a splitting of the $E_0$ transition into a light hole-like transition (lh) and a heavy hole-like transition (hh). The energy separation between these two transitions is given by $2b(1+2C_{12}/C_{11})\varepsilon$, where $\varepsilon$ is the in-plane strain and $C_{ij}$ the elastic moduli. Strain also induces an energy shift on the center of gravity of the two, hh and lh, transitions being its magnitude $2a(1-C_{12}/C_{11})\varepsilon$. If the strain is tensile (as it is in this work) the lh transition is located at lower energy, whereas a compressive strain the hh transition appears at lower energy.

For the $E_1$ and $E_1$ transitions, as they occur between states along the (111) directions, a biaxial strain of the present characteristics does not produce any splitting but a modification of the energy separation between $E_1$ and $E_1+\Delta_1$, given by $[\Delta_1^2 + (8/3)D_3^2(1+C_{12}/C_{11})^2\varepsilon^2]^{1/2}$, where $\Delta_1$ is the spin-orbit splitting and $D_3$ the intraband deformation potentials.
The deformation potential for the $\Lambda_2$ valence band under [001] uniaxial strain. There is also a shift of the energy of the center of gravity of the two transitions given by $2\varepsilon_1(1-C_{12}/C_{11})\varepsilon$ where $\varepsilon_1$ is the hydrostatic interband $(\Lambda_3-\Lambda_1)$ deformation potential.

If the strain field is known, the measurement of the splitting between $h$ and $l$ transitions directly gives the shear deformation potential $h$, whereas the determination of $D^3_3$ requires the knowledge of the spin-orbit splitting. The determination of the hydrostatic deformation potentials $a$ and $\varepsilon_1$, requires the knowledge of the energy of the $E_0$ and $E_1$ transitions at zero strain, respectively.

In Fig. 1 we show the electroreflectance spectra obtained in the $E_1$ region and in Fig. 2 those obtained in the $E_0$ region. The points are the experimental data and the full curves a theoretical fit using third derivatives functional forms. As expected, the strain produces a splitting of the fundamental transition into $l$-like and $h$-like transitions. In our experimental configuration, with the incident and reflected light polarized in the (001) plane, the intensity of the $l$-like transition should be three times lower than the intensity of the $h$-like transition, as it is observed. The energies obtained with these fits are given in Table I.

Once we have experimentally determined the modification of the $E_0$ and $E_1$ transitions dependence on strain, previously obtained by DCXRD characterization, we can directly obtained the deformation potentials values by using the above referred expressions. The energy of the $E_0$ and $E_1$ transitions at zero strain have been taken from Ref. 9. The values of the deformation potentials obtained in this way are shown in Table I. In Table II we show the deformation potential of the binary compounds. Due to the strong dispersion in the experimental values of the deformation potentials of the binary compounds, it is difficult to establish any evo-
TABLE I. Double crystal x-ray diffraction determined compositions (x) and residual strain (ε) as well as the thickness (d) of the GaAs₁₋ₓPₓ samples studied in this work are shown in this table. E₀, E₁, D₁, and E₁+Δ₁ are the energies of the optical transitions obtained from electroreflectance spectra at T=80 K by using a theoretical fit with third derivative functional forms and the obtained values of the deformation potentials.

<table>
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<th>x</th>
<th>0.2</th>
<th>0.24</th>
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<tr>
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<td>400</td>
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<td>E₀ (eV)</td>
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<td>-5</td>
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In summary we have studied the electroreflectance spectra of a series of GaAs₁₋ₓPₓ samples grown by ALMBE on GaAs substrates, with an approximately constant P composition (0.20≤x≤0.24) and different layer thicknesses. Due to the lattice mismatch relaxation dependence on layer thickness, the residual strain in the GaAs₁₋ₓPₓ layers changes from one sample to another, and this fact allows us to determine the hydrostatic and shear deformation potentials of the E₀ and E₁ transitions of GaAs₁₋ₓPₓ for a composition x=0.20.

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