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LETTER TO THE EDITOR

Elastic constants of $In_xGa_{1-x}As$ and $In_xGa_{1-x}P$ determined using surface acoustic waves

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Abstract. The elastic constant tensors of thin layers of $In_xGa_{1-x}As$ and $In_xGa_{1-x}P$ with compositions around $x = 0.5$ have been determined using surface acoustic waves measured by Brillouin light scattering spectroscopy. Contrary to the case for the usual estimates, the experimentally obtained elastic constants are different from the ones calculated by simple linear combination of those of the corresponding constituent binary compounds. An averaging model combining a parallel–serial disposition of springs with the elastic constants corresponding to the binary compounds has been used to explain the elastic constants of the ternary alloys. This model explains perfectly the elastic properties of the $In_xGa_{1-x}As$ system, while those of the $In_xGa_{1-x}P$ system are not reproduced.

The method generally used in the literature for determining the elastic constant tensors (C_{ij}) of alloys usually consists in simple linear combination of those of the constituent components [1]. This method has been employed for ternary alkali halides whose elastic constants were used as input parameters for studying their hardness [2]. Recently, Krieger and Sigg [3] found in a Brillouin light scattering (BLS) spectroscopy study of the $Al_{1-x}Ga_xAs$ system that its elastic constant tensor differs slightly from that calculated by linear interpolation of the binaries' C_{ij}. From such results it can be deduced that the method generally used for calculating the ternary alloys' C_{ij} by linear combination of those of its binary components could be inexact, because the requirement of linearity of the elastic constant behaviour is not fulfilled.

We have studied two III–V systems: $In_xGa_{1-x}As$ and $In_xGa_{1-x}P$ with compositions around $x = 0.5$. Our aim was twofold: to report their elastic constant tensors, and to investigate the effect on their elastic behaviour of the observed differences in the optical [4] and relaxation [5, 6] properties.

These alloys present modulation composition features related to the existence of a miscibility gap. In particular, in transmission electron microscopy studies [5] strong dark and bright fringes can be seen, which are associated with regions of slightly different compositions. In order to assess the influence of changes in the structural features on the elastic behaviour, near-lattice-matched samples 1 μm thick have been grown by atomic-layer molecular beam epitaxy [7] (ALMBE). The samples studied are: $In_{0.49}Ga_{0.51}As/InP(001)$ and $In_{0.53}Ga_{0.47}As/InP(001)$, grown in As-rich and InGa-rich atmospheres, respectively; and $In_{0.47}Ga_{0.53}P/GaAs(001)$ and $In_{0.49}Ga_{0.51}P/GaAs(001)$, grown in P-rich and InGa-rich atmospheres, respectively.

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BLS experiments were carried out using a 3 + 3 tandem Sandercock-type [8] spectrometer. Standard backscattering geometry was used to determine the phase velocity of the Rayleigh-type surface phonons [9].

The results were fitted using a simulation program that permits calculation of the Brillouin spectrum of a layer/substrate system [10] using as input the densities and C_{ij} of the layer and substrate. As the layer is an alloy, the density for simulations was obtained through Vegard's law. This law is an approximation used to predict a physical magnitude for a binary alloy, which is based on an interpolation between the values for the constituent elements. $In_xGa_{1-x}As$ (and consequently $In_xGa_{1-x}P$) alloy can be considered as a binary alloy of the two well known compounds InAs and GaAs. Vegard's law provides a density (ρ) for $In_xGa_{1-x}As$ that can be calculated as

$$\rho_{InGaAs} = x\rho_{InAs} + (1-x)\rho_{GaAs}.$$

At this point, the three independent elastic constants of the layer were varied until the mismatch between the patterns and the experimental points was minimized. The sensitivity in the determination of C_{ij}-values by this fitting method is around 1 GPa for all of the samples. In figure 1, the experimentally obtained phonon velocities of the $In_{0.49}Ga_{0.51}P$ (InGa-rich) sample and their simulations are presented, as determined in an azimuthal experiment.

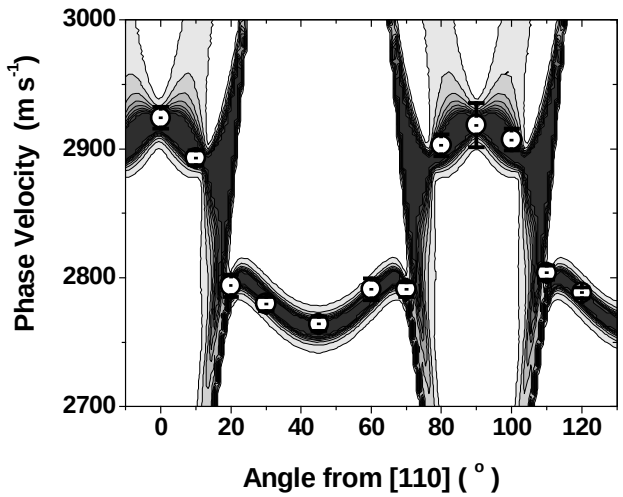

Figure 1. A contour plot of the azimuthal dispersion of the Rayleigh phonon phase velocity for $In_{0.49}Ga_{0.51}P$ (an InGa-rich sample). Circles represent the experimental points while contours correspond to the simulation. The error bars of the experimental points have been obtained from the Brillouin peak position uncertainties.

It is well known that the elastic constants of opaque materials obtained by BLS are different and slightly lower than those measured by ultrasound techniques [11]. We measured the C_{ij} of the four binary compounds (InAs, GaAs, InP and GaP) before drawing any conclusions from the ternary's results. Once the binaries' C_{ij} were measured we used linear combination (LC) as a starting point for the ternaries fits. After verifying that linear combination could not satisfactorily produce the experimental values, we generated a different method of averaging the elastic constants based on physical grounds.

On the basis of the observed columnar structure, which is similar for both As and P alloys [5, 6], we propose the averaging model that is shown schematically in the inset of figure 2. In this simple model, hereafter called the columnar-averaging model, the system can be described

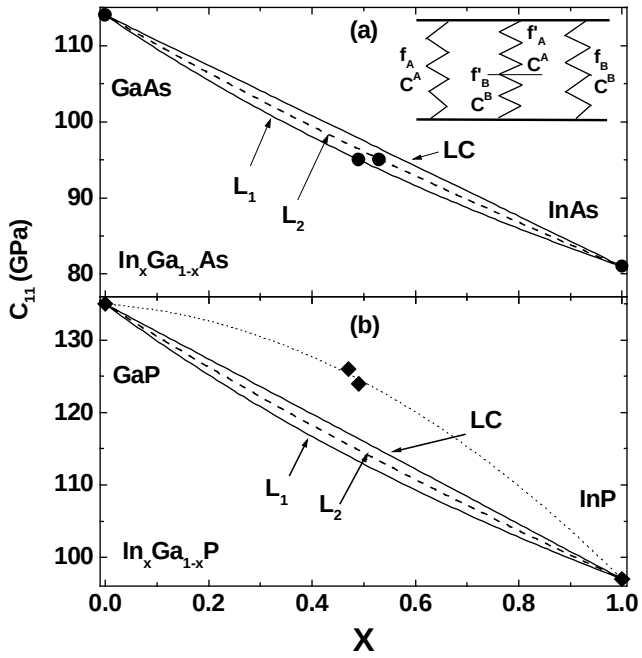

Figure 2. Experimental values (points) and the results of different averaging calculations of the elastic constant C_{11} for (a) $In_xGa_{1-x}As$ and (b) $In_xGa_{1-x}P$ as functions of the composition x. The inset shows a schematic spring representation of the elastic constant columnar-averaging model.

as an association of springs with elastic constants C^A and C^B, corresponding to each of the binaries' elastic constant tensors. The springs are set in a serial–parallel combination as follows: there exists a zone in which there is only a contribution of binary type A (C^A) with a certain weight f_A; then there is a zone in which there is a combination of materials of type A and B in a serial association with respective fractions f'_A and f'_B (thus having a total weight $f'_A + f'_B$); and finally there is a third column in which only material of type B with fraction f_B contributes to the total elastic constant tensor. Taking into account this material disposition, the elastic constant tensor of the ternary $In_xGa_{1-x}As$ (or $In_xGa_{1-x}P$) alloy will be

$$C = f_A C^A + (f'_A + f'_B)\left(\frac{f'_A}{(f'_A + f'_B)C^A} + \frac{f'_B}{(f'_A + f'_B)C^B}\right)^{-1} + f_B C^B \qquad (1)$$

with $f_A + f'_A = x$ and $f_B + f'_B = 1 - x$, where x gives the relative concentration of the binaries.

The two extremes of such a model will correspond to a serial-spring association, in which $f_A = f_B = 0$ (which is the lower limit for the calculated elastic constant), and a parallel-spring association, in which $f'_A = f'_B = 0$ (which is the upper limit and which formally is the linear combination).

In table 1, the experimental elastic constant values can be compared with those obtained for an intermediate situation, columnar averaged, where $f_A + f'_A = x/2$ and $f_B + f'_B = (1-x)/2$.

Figure 2 shows the experimental values (points) of the elastic constant C_{11} for $In_xGa_{1-x}As$ and $In_xGa_{1-x}P$ as functions of the composition x. Along with them, several curves are presented. The curve marked LC corresponds to the linear combination. Curve L_1 corresponds to the lower limit of the columnar average, while L_2 (the dashed curve) represents a situation where $f_A + f'_A = x/2$ and $f_B + f'_B = (1-x)/2$. In figure 2(b), a curve drawn by eye (the dotted curve) has been included to show a possible compositional dependence of the elastic

Table 1. Experimental elastic constant values and values for the ternary alloys calculated (marked with asterisks) using the columnar-averaging method.

Sample	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
InAs	81 ± 1	44 ± 1	39 ± 1
GaAs	114 ± 1	52 ± 1	57 ± 1
InP	97 ± 1	54 ± 1	45 ± 1
GaP	135 ± 1	60 ± 1	67 ± 1
$In_{0.49}Ga_{0.51}As$	95 ± 1	48 ± 1	45 ± 1
	97.8*	48.0*	47.9*
$In_{0.53}Ga_{0.47}As$	95 ± 1	49 ± 1	45 ± 1
	96.5*	47.7*	47.2*
$In_{0.47}Ga_{0.53}P$	126 ± 1	63 ± 1	60 ± 1
	116.8*	57.4*	56.6*
$In_{0.49}Ga_{0.51}P$	124 ± 1	62 ± 1	59 ± 1
	116.0*	57.3*	56.1*

constant C_{11} of $In_xGa_{1-x}P$.

Several things should be noted: we have shown that linear combination is not sufficient to reproduce the elastic constant values of these III–V ternary alloys. Thus, in future, some care should be taken when obtaining the C_{ij} of different alloy compositions in order to use them in other kinds of calculation. The behaviour of the elastic constants of the layers does not depend on the growth conditions, showing similar values for samples grown in either 'III-rich' or 'V-rich' atmospheres. This implies that the period of the modulation of the composition is not relevant to the elastic behaviour.

We have established that the 'columnar-average' approaches could satisfactorily reproduce, within the experimental errors, the elastic constant values of the In–Ga–As samples. On the other hand, the elastic constants of the In–Ga–P system cannot be explained within the framework of the 'columnar-average' model; in fact, the elastic constants are up to 12% higher than the linear combination values. Taking into account that the elastic constants of In–Ga–As are lower than those calculated by linear combination, there exists a non-negligible difference in the elastic behaviour of these III–V alloys. The cause of this difference could have a structural origin, such as the accumulated strain [12]. However, x-ray diffraction characterization shows that the strains of these layers are small and very similar (below 2×10^{-3}). The reason for such a different behaviour could then be differences in the bonding nature of the binaries constituting In–Ga–As and In–Ga–P. Some first-principles calculations should be performed in order to verify the validity of such an explanation.

In conclusion, the elastic constants of the systems $In_xGa_{1-x}As$ and $In_xGa_{1-x}P$ with compositions around $x = 0.5$ have been determined for the first time using the surface acoustic waves measured by Brillouin light scattering spectroscopy. The elastic constant tensors of these III–V semiconductor ternary compounds cannot be explained on the basis of a simple linear combination of those of their corresponding constituent binaries, which has been the method generally used up to the present. A new averaging model called the columnar-averaging model

has been employed for these specific systems; it is based upon structural information. This averaging procedure reproduces the elastic constant tensor of the In–Ga–As alloy. In contrast, the elastic properties of the In–Ga–P alloy cannot be reproduced either by linear combination or by columnar averaging. The difference between the behaviours of the elastic constants for the two ternaries could be attributable to the different bonding potentials involved for $In_xGa_{1-x}As$ and $In_xGa_{1-x}P$ alloys.

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