Interfacial Layers and Impurity Segregation in $InP/In_{0.53}Ga_{0.47}As$ Superlattices

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The interfaces in $InP/In_{0.53}Ga_{0.47}As$ superlattices modulation doped with Si were investigated using magneto-transport, capacitance-voltage, and high resolution X-ray diffraction measurements. Results indicate that a thick interfacial layer is formed when InP is grown on top of $In_xGa_{1-x}As$, and that Si atoms that fall in the interfacial layer have a high probability of not forming a shallow donor center. Using a simple theoretical model the width of the interfacial layer which was estimated to be 7 ± 1 monolayers.

I Introduction

The ability to produce abrupt interfaces between epitaxial layers is important in manufacturing modern optoeletronic devices, because graded interfaces can disrupt the optical spectra [1] and reduce carrier mobility [2], hindering device applications [3]. For this reason, many efforts have been spent to attain abrupt interfaces in heterostructures.

To improve interfaces, a commonly used procedure consists in an interruption of the growth process between the growth of two different layers [4]-[10]. For $InP/In_{0.53}Ga_{0.47}As$ systems grown by metalorganic vapour phase epitaxy, during growth interruption the growth chamber is kept under a flow of the group V element (P, As) of the layer to be grown subsequently. For interruption times of ~1s, the interface between $In_{0.53}Ga_{0.47}As$ grown on InP (the so-called *upper* interface) is abrupt [5, 6]. However, an adequate procedure to obtain an abrupt interface for InP grown on $In_{0.53}Ga_{0.47}As$ (the so-called *lower* interface) has not been reported yet. The lower interface is always graded, and contains an interfacial layer of chemical composition $InAs_xP_{1-x}$. The interfacial layer occupies the space which in an ideal structure would be occupied by pure InP and the thickness and the chemical composition of the interfacial layer are very sensitive to the growth conditions [5]-[10]. To establish the ideal growth conditions, reliable experimental procedures to characterize the interfaces are needed. However, this is a difficult task, due to the limitations inherent to the techniques used traditionally for that purpose, i.e. high resolution X-ray diffraction (HRXRD) and SIMS [7]. From HRXRD measurements on short period superlattices, when the X-ray spectra show few satellite peaks, the thickness and the strain of the interfacial layer cannot be established independently, only the product of these quantities can be determined [8]. SIMS measurements are limited in resolution due to crater curvature and the knock-on effect [11], and cannot be used to deduce the thickness of an individual layer with an accuracy greater than ±15Å[10].

In this work we present a study of the interfaces in $InP/In_{0.53}Ga_{0.47}As$ superlattices using a combination of HRXRD, capacitance-voltage (C-V) and magneto-transport measurements. The analysis of the entirety of the results obtained allows us to estimate the thickness of the interfacial layer at the lower interface to be 6-8 monolayers (ML) (1 monolayer ~ 3 Å) in our samples.

II Experimental procedure

$InP/In_{0.53}Ga_{0.47}As$ superlattices modulation doped with Si in the middle of InP barriers were grown by low pressure metalorganic vapor phase epitaxy (LP-MOVPE). Growth was interrupted at the interfaces for 1 s, during this time interval the growth chamber was kept under the flow of group V element of the layer to be deposited subsequently, in accordance to the prescription which yielded the best interfaces reported so far. The growth procedures of the samples are described in details in Ref. [12]. All the samples had the same thick-

ness of the $In_{0.53}Ga_{0.47}As$ layers (50Å), but differed in the thickness of the InP layers and in the doping level. Further details on the experimental techniques used can be found in Ref. [13].

III Results and discussion

In order to determine the characteristic width of the layers doped with Si in our samples, the C-V spectrum of the control sample 311 was measured, which consists of a thick InP layer containing a single crystalline plane doped with Si (delta-doped layer). The C-V spectrum was reproduced theoretically following the prescription described in Ref. [14]. Fig. (1) shows the experimental and theoretical C-V spectra, which determine that the Si atoms are distributed in a layer whose characteristic width is w = 18 Å (6 ML). The non-zero thickness of the Si layer is a consequence of impurity segregation during the growth process, whereas diffusion is negligible [15]. The thickness w=6 ML shows that in our samples Si segregation is much less effective than found by Skuras *et al* [15] in samples grown by MBE, whereby the characteristic width of the doped layer was found to be 45 ML.

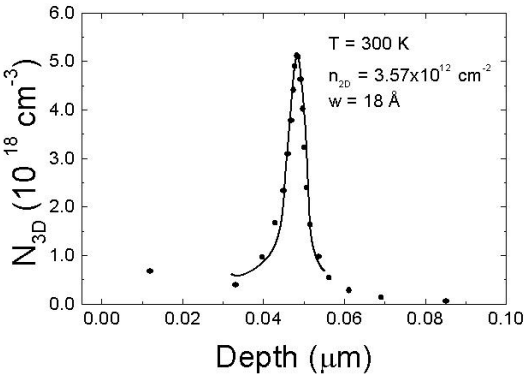

Figure 1. C-V spectrum of sample 311. The squares are the experimental data and the solid line is the theoretical curve.

The superlattice period of the samples was obtained from their HRXRD spectra; the thickness of the InP layers was obtained by subtracting the nominal thickness of the $In_{0.53}Ga_{0.47}As$ from the superlattice period. The density of free carriers was deduced from a two carrier fit to the magnetoresistance data. Table 1 summarizes the results. The value of N_d given in Table 1 corresponds to the nominal value of the areal density of active Si atoms in each InP barrier, which was derived from the Shubnikov-de Haas spectra of delta-doped layers grown under the same conditions. Table 1 shows that the density of free carriers decreases with the thickness of the InP layers. For narrow barriers, the probability that a given Si atom falls into an interfacial layer is greater than for thicker ones. Thus the observed decrease in the density of free carriers correlates with the number of Si atoms that are located in the interfacial layers. This suggests that the Si atoms at the interfaces are not electrically active. The possibility thatthese Si atoms form shallow complexes is also excluded, given that the measured density of free carriers does not display activated behavior in the 2-300 K temperature range. A possible explanation is that some of the Si atoms located within the interfacial layers form negatively charged DX^- centers [16, 17]. The disorder and mechanical strain, which are present at the interfaces [9] favor the formation of DX centers[17].

Table I. Sample parameters obtained from Shubnikov-de Haas spectra. n_s is the sheet carrier density and N_d is the nominal doping density.

Sample	InP layer width (Å)	n_s (10^{12}cm^{-2})	N_d (10^{12}cm^{-2})	n_s/N_d
311	-	3.95	3.95	1.000 ± 0.006
327	48.5	4.205	5.34	0.79 ± 0.06
326	47.5	3.242	3.95	0.82 ± 0.06
331	40.7	3.389	5.34	0.63 ± 0.05
332	38.2	2.593	3.95	0.66 ± 0.05
333	28.9	1.611	3.95	0.41 ± 0.04
334	28.1	1.815	5.34	0.34 ± 0.04
336	20	1.106	3.95	0.28 ± 0.04
335	17.8	1.668	5.34	0.31 ± 0.04

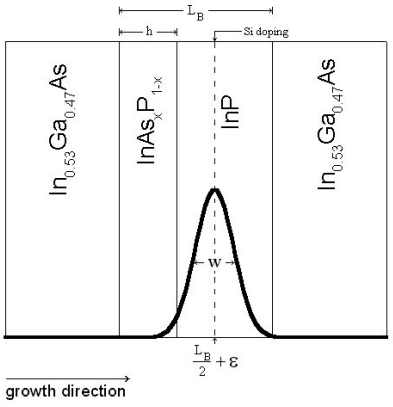

Figure 2. A Si planar doped $InP/In_{0.53}Ga_{0.47}As$ superlattice with an interface layer of $InAs_xP_{1-x}$ (with width h), between InP grown on $In_{0.53}Ga_{0.47}As$.

To model theoretically the reduction of free carriers when the thickness of InP barriers decreases, we will assume that the upper interface is ideal, whereas the lower one is graded, with an interfacial layer of thickness h. The Si atoms are supposed to be distributed statistically along the growth axis in accordance with a Gaussian of full width of half maximum equal to the characteristic width of the doping layer, i.e. w = 6 ML. Due to the segregation effect, the center of the Gaussian is allowed to be displaced from the center of the InP barriers, by the segregation length, ε. Fig. (2) shows schematically the epitaxial layers, the interfacial layer and the statistical distribution of Si atoms. We assume that a given Si atom has a probability p of forming a charged DX^- center [11], when it falls within the interfacial layer, thus binding two electrons. In this case

the amount of free carriers, as a function of the barrier width, L_B, is given by:

$$\frac{n_s}{N_d} = 1 - p\left\{\mathrm{erf}\left[\frac{\sqrt{4\ln 2}}{w}\left(\frac{L_B}{2} + (h - L_B)\Theta(L_B - h) - \varepsilon\right)\right] - \mathrm{erf}\left[\frac{\sqrt{4\ln 2}}{w}\left(-\frac{L_B}{2} - \varepsilon\right)\right]\right\} \quad (1)$$

where N_d is the areal density of Si atoms introduced into each of the InP barriers, $\Theta(x) = 1$ if $x > 0$; and $\Theta(x) = 0$ if $x < 0$, and $\mathrm{erf}(x)$ is the error function:

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-u^2} du \quad (2)$$

Fig. (3) shows the experimental data and the best theoretical fit using Eq. (1), whereby the fitting parameters are h, p, and ε. For the dotted curve, segregation was not allowed for and ε was fixed at zero; this produces a lower bound estimate of the thickness of the interfacial layer, which is found to be h =6 ML, for $p = 0.51$. For the continuous curve, ε was free to adjust itself, resulting in ε =1 ML, an interfacial layer of 7 ± 1 ML, and $p = 0.48 \pm 0.05$. The small value of ε obtained is supportive of our earlier conclusion that the segregation effect is practically absent in the samples used in this work.

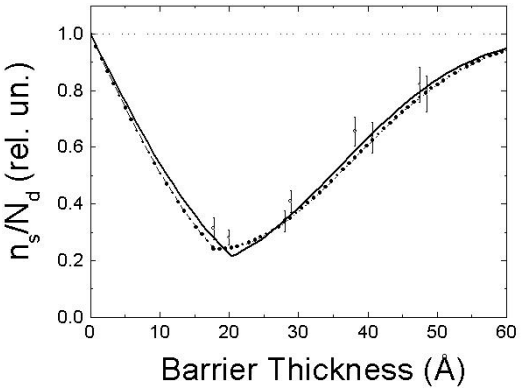

Figure 3. Experimental data and model curves given by Equation 1, with $\varepsilon = 0$ (doted curve) and $\varepsilon = 1$ ML (solid curve).

Using the analysis of HRXRD measurements, Jiang et. al. [9] estimated that for a $In_{0.53}Ga_{0.47}As$/ InP (112Å/36Å) superlattice, the lower interface layer is of $InAs_{0.28}P_{0.72}$ composition, with a thickness of 12 ML. The sample studied was grown under very similar conditions to the ones used by us. Jiang [9] suggested that the thickness of the interfacial layer increases with the amount of residual As in the growth chamber. The amount of As in the growth chamber increases with the thickness of the $In_{0.53}Ga_{0.47}As$ layer just grown. From the data reported by Jiang and co-workers [9], it can be deduced that the width of the interfacial layer is of the order of 5.3 ML for every 50 Å of $In_{0.53}Ga_{0.47}As$. This result is quite similar to the one obtained by us for our samples, all of which had the same thickness of 50Å in the $In_{0.53}Ga_{0.47}As$ layers, and whose interfacial layer we estimated to be of thickness 7 ML.

Further support to the conclusion that our samples contain a thick lower interface can be seen in Fig. (4), which depicts a typical HRXRD spectrum for our samples. The HRXRD spectrum exhibits satellite peaks of order +2, +3, and +4 much less intense than the peaks of order -2, -3, and -4, respectively, which is aditional evidence of the presence of an interfacial layer [9].

IV Conclusions

It was found that the density of free carriers in modulation-doped $InP/In_{0.53}Ga_{0.47}As$ superlattices decreases very rapidly when the width of the InP layers in the structure decreases. The reduction in the free carrier density correlates with the number of doping atoms which fall in the interfacial layer formed when InP is grown on top of $In_xGa_{1-x}As$. Using the transport data and assuming the spatial distribution of the Si atoms to be as deduced from C-V measurements, the thickness of the interfacial layer was estimated. A simple theoretical model was developed, in which it is assumed that the doping atoms can be inactive when they are located within an interfacial layer. Using this model the width of the interfacial layer was estimated to be ∼7 ML. To determine the exact fate of the Si atoms that fall in the interfacial layer further investigations are required. The model also indicates that the segregation length of Si is very small (≤1 ML) in our samples.

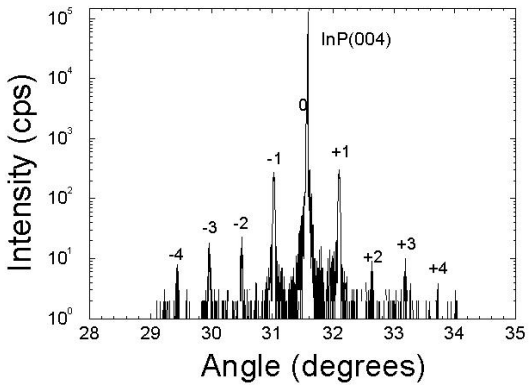

Figure 4. X-ray spectrum of sample 326.

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