FIR REFLECTIVITY SPECTRA OF A THICK SUPERLATTICE WITH A BUFFER LAYER

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Abstract

Infrared reflectivity spectra of GaAs/AlGaAs thick multiple heterostructures in the far infrared range up to 450 cm^{-1} have been investigated. A large influence of the buffer layer in the transparency region between the two "Reststrahlen" bands, of GaAs and AlAs, is observed. It was shown that a simple analysis of experimental data with an iterative method, performed in the effective medium approximation, allows a very accurate determination of the structural parameters not only of the SL but also of the buffer layer.

1 Introduction

Many optoelectronic devices, such as semiconductor lasers diodes, detectors, modulators and non–linear optical devices are based on multilayered structures composed of various thin homo– or heterolayers of different thicknesses and doping levels.

The characterization of electrical and structural parameters, such as the layer thicknesses and the composition concentration, x, of these complex structures is a challenge.

Far–infrared reflectivity (FIR) is a non–destructive, non–contact method of characterizing both structural and transport properties of layerd structures. It has been demonstrated that the "Reststrahlen" bands appearing in the FIR spectra are mainly influenced by the ratio $\rho = d_1/d_2$ between the individual layer thicknesses [1]. The use of FIR for structural characterization of SL has already been proposed [2].

In this work we investigate the reflectivity spectra of a GaAs/Al_xGa_{1-x}As in the FIR region 150–450cm^{-1}. Our analysis demonstrates that not only the structural properties of the superlattice, total thickness and individual layer thicknesses d_1/d_2, but the structural properties of the buffer layer, $\approx 8\mu m$ below the top of the structure, can be characterised with a good accuracy.

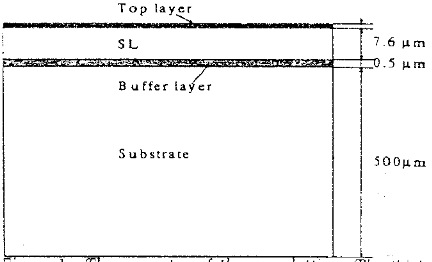

Figure 1: *The geometry of the superlattice. The thickness of the top layer is 500 Å.*

2 Theory

A standard problem in thin–film optics [4] is the calculation of the reflecitivity for the geometry shown on Fig.1 when the superlattice is described in the average–medium approximation [3]. The electric field in medium n for normal incidence can be expresed:

$$E_n(z) = E_n^+ \exp(ik_n z) + E_n^- \exp(-ik_n z), \qquad (1)$$

where $k_n^2 = \epsilon_n (2\pi\omega)^2$, and for our system $n = 1 \ldots 4$, ϵ_1 and ϵ_4 are the dielectric functions for GaAs topmost layer and substrate, ϵ_2 the dielectric function for normal incidence on the superlattice and ϵ_3 the dielectric function for the $Al_xGa_{1-x}As$ buffer layer. The complex ratio of the total amplitude in the $-z$ direction to that in the $+z$ direction could be written with the following relation:

$$R_{n-1,n} = E_n^- / E_n^+, \qquad (2)$$

For a multiple layer system application of standard boundary conditions gives an effective complex reflection coefficient for the n–layer

$$R_{n-1,n} = \frac{r_{n-1,n} + R_{n,n+1} \exp(2ik_n d_n)}{1 + r_{n-1,n} R_{n,n+1} \exp(2ik_n d_n)}, \qquad (3)$$

where d_n is the thickness of the n-the layer, and

$$r_{n-1,n} = \frac{\sqrt{\epsilon_{n-1}} - \sqrt{\epsilon_n}}{\sqrt{\epsilon_{n-1}} + \sqrt{\epsilon_n}}, \tag{4}$$

is the complex reflection coefficient for an isolated $n-1$ to n interface. If we assume that the GaAs substratum is semiinfinite, there is no wave propagating in the $-z$ direction in medium 4, so $R_{3,4} = 0$. With this condition equation (4) can be iterated to determine the complex reflection coefficient of the system. The reflectivity of the structure can be easily calculated from:

$$R = |R_{0,1}|^2 \tag{5}$$

The well known equation for the reflectivity of a superlattice on a bulk substrate, derived from relations given by O. Piro [5], and first presented by Scamarcio et.al.[1] can be easily derived using our iterative method. For normal incidence of light, which is in our case, s and p polarizations are indentical. To derive this equation we will assume that the thicknesses of the upper layer and the buffer layer are zero. After these assumptions we get the following system of equations:

$$R_{0,1} = \frac{r_{0,1} + R_{1,2} \exp 2ik_1 d_1}{1 + r_{0,1} R_{1,2} \exp 2ik_1 d_1}, \tag{6}$$

$$R_{1,2} = r_{1,2}, \tag{7}$$

$$r_{0,1} = \frac{1 - \sqrt{\epsilon_1}}{\sqrt{1} + \sqrt{\epsilon_1}}, \tag{8}$$

$$r_{1,2} = \frac{\sqrt{\epsilon_1} - \sqrt{\epsilon_2}}{\sqrt{\epsilon_1} + \sqrt{\epsilon_2}}. \tag{9}$$

Index "0" stands for air or vacuum, where we can assume that $\epsilon_0 = 1$. "1" stands for the superlattice, $d_1 = d_{sl}$, $\epsilon_1 = \epsilon_{sl}$ and "2" for the substrate, $\epsilon_2 = \epsilon_b$. After some tedious and straitforward mathematics we come to the following, well known equation:

$$R = \left| \frac{\left(1 - \frac{1}{\sqrt{\epsilon_b}}\right)\cos(\alpha) - i\left(\sqrt{\frac{\epsilon_{sl}}{\epsilon_b}} - \frac{1}{\sqrt{\epsilon_{sl}}}\right)\sin(\alpha)}{\left(1 + \frac{1}{\sqrt{\epsilon_b}}\right)\cos(\alpha) - i\left(\sqrt{\frac{\epsilon_{sl}}{\epsilon_b}} + \frac{1}{\sqrt{\epsilon_{sl}}}\right)\sin(\alpha)} \right|^2 \tag{10}$$

where $\alpha = 2\pi i w \sqrt{\epsilon_{sl}}$.

The dielectric function of the superlattice, in the long-wavelength limit, can be determined using a average-medium description [3]. In the case of normal incidence the electric field E is parallel to the layers and the dielectric function can be written in the following form:

$$\epsilon_{sl}(\omega) = \frac{\rho\epsilon_1(\omega) + \epsilon_2(\omega)}{\rho + 1} \tag{11}$$

where $\rho = d_1/d_2$, is the ratio of the layer thicknesses, ϵ_1 and ϵ_2 are the dielectric functions of material "1" (GaAs) and "2" ($Al_xGa_{1-x}As$), respectively. In the framework of a classical oscillator model ϵ has the form:

$$\epsilon(\omega) = \epsilon_\infty + \sum \frac{2\pi\rho\omega_{TO}^2}{\omega^2 - \omega_{TO}^2 - i\omega\Gamma_{TO}} \tag{12}$$

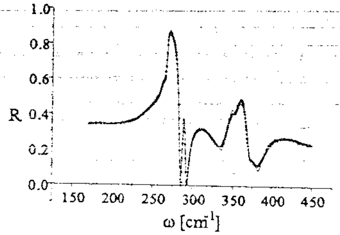

Figure 2: *The FIR reflectivity spectra. Experimental results (*), calculated full line and calculated without the buffer layer dotted line*

in the three parameter model and:

$$\epsilon(\omega) = \epsilon_\infty \prod \frac{\omega^2 - \omega_{LO}^2 - i\omega\Gamma_{LO}}{\omega^2 - \omega_{TO}^2 - i\omega\Gamma_{TO}} \tag{13}$$

in the four parameter, or factorized model. ϵ_∞ stands for the high-frequency dielectric permitivity, $2\pi\rho = \epsilon_0 - \epsilon_\infty$ the oscillator strength, ω_{TO} and ω_{LO} the transverse and longitudinal-optical phonon frequency, respectively, Γ_{TO} and Γ_{LO} are the phenomenological damping factor for transverse and longitudinal-optic phonons.

3 Experimental results

The GaAs – $Al_{1-x}Ga_xAs$ superlattice were grown by molecular-beam epitaxy (MBE) on (100) GaAs substrates at Department of Physics, Nottingham University. Growth was performed at a substrate temperature of 580°C which was later increased to 630°C. The superlattice details are given Table 1. Reflection measurements at near-normal incidence were made in two ranges: FIR from 50 to 450 cm^{-1} with a Fourier spectrometer, Brucker 113V, located at the Aristotel University of Thesalonikee. The spectra were taken with 0.5 cm^{-1} resolution in the FIR.

4 Results and discussion

Our sample shown in Fig.1, consists of a very thin GaAs, $d_t = 200$ Å, layer on top of a superlattice, which consists of an alternating slabs of GaAs, $d_1 = 101.7$ Å thick, and $Al_{1-x}Ga_xAs$, $d_2 = 152$ Å thick, with $x = 0.33$. Between the superlattice and the semi-insulating GaAs, substratum there is a buffer layer of $Al_{1-x}Ga_xAs$, with the same composition as in the superlattice.

The far infrared reflectance spectrum is shown in Fig. 2 and it is seen to contain several interesting features. Firstly, wee can see that the spectra is dominated by two reststrahlen bands, near 270 cm^{-1} a strong GaAs and a weak AlAs near 375 cm−1. Secondly, the GaAs reststrahlen band has a shoulder on the low-energy side

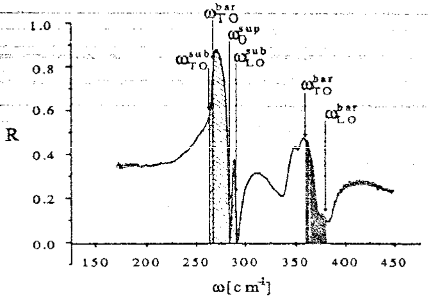

Figure 3: *The FIR reflectivity spectra showing regions with negative values of ϵ.*

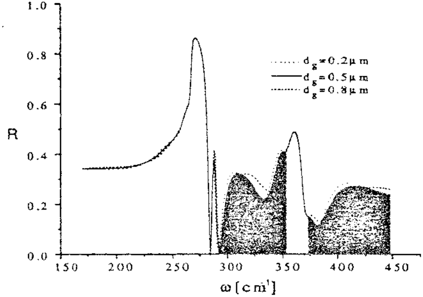

Figure 4: *The FIR reflectivity spectra showing the influence of the buffer layer.*

and a sharp dip near 280 cm^{-1}. The shoulder is a consequence of the influence of the GaAs–like mode of the AlGaAs from the superlattice. In this work it is shown that the influence of the buffer layer should not be neglected even more must be tacken into account. The dip near 280 cm^{-1} has a more complex origin.

Within the GaAs optic region, the spectra are dominated by the response of the substrate, producing the rise in reflectivity around the bulk TO frequency 268 cm^{-1} and a sharp cutoff above the bulk LO frequency 292 cm^{-1}. The dip near 280 cm^{-1} is due to interference between the top and bottom surface of the superlattice, and occurs in the region where ϵ_{sl} for the superlattice is positive but ϵ for the GaAs substrate is negative. Most of the radiation passing through the superlattice in this frequency region is therefore reflected by the substrate, so the reflected signal consist also of two transmissions through the superlattice. A dip in the spectrum appears because a portion of the light is absorbed by the superlattice. The position of the dip is in good agreement with the value were $\epsilon_{sl} = 0.3$.

On 4 we show the FIR reflectivity spectra togather with the regions with negative values of the dielectric function for the superlattice, substrate and buffer layer.

In table 1. we summarize the values obtained by a fit-

Table 1: Oscillator parameters obtained from the curve fitting by using a factorized and a additive form of a dielectric function.

	factorized	S& K[a]	additive	S& K[b]
GaAs substrate				
ε_∞	11.1	10.9	11.1	10.9
$4\pi\rho$	-	-	2.04	2.03
ω_{TO}	268.3	268.8	269.0	269.2
γ_{TO}	2.43	2.65	3.48	2.5
ω_{LO}	291.5	292.8	-	292.8
γ_{LO}	2.363	2.85	-	-
GaAs wells				
ε_∞	11.8	10.9	13.	10.9
ω_{TO}	267.9	268.8	268.1	269.2
γ_{TO}	2.08	2.65	1.64	2.5
ω_{LO}	291.9	292.8	-	292.8
γ_{LO}	2.46	2.85	-	292.8
$4\pi\rho$	-	-	2.00	2.03
AlGaAs barrier and buffer				
GaAs like				
ε_∞	10.0	10.08	9.1	10.1
ω_{TO}	264.3	264.85	264.3	264.7
γ_{TO}	7.75	9.64	4.88	7.45
ω_{LO}	277.2	277.4	-	276.9
γ_{LO}	5.03	5.86	-	-
$4\pi\rho$	-	-	1.29	1.16
AlGaAs like				
ω_{TO}	359.5	360.3	359.5	360.9
γ_{TO}	9.25	12.17	10.45	10.5
ω_{LO}	376.5	380.1	-	379.8
γ_{LO}	10.0	8.75	-	-
$4\pi\rho$	-	-	0.93	0.97
$\rho = d_1/d_2$	0.68	0.66	0.72	-
$D_{sup}[\mu m]$	7.8	7.65	7.93	-
D_{buf}min	0.545	0.5	0.447	-

[a] FIR on $Al_xGa_{-x}As$ alloys. factorized form (Kim and Spitzer. Ref[6]

[b] FIR on $Al_xGa_{-x}As$ alloys. additive form (Kim and Spitzer. Ref[6]

ting procedure using the presented iterative model. The obtained values both for three and four parameter model are in very good agreement with the literature values [6]. The parameters for the buffer layer were not fitted separately. It was noriced that they had the same values as the parameters for the $Al_xGa_{1-x}As$ layer from the superlattice, as expected. The only discrepancy between our results and the known ones [6] is for the value of the ω_{LO} frequency of the AlAs-like phonons from the $Al_xGa_{1-x}As$. This could be due to the influence of the cation interdiffusion at the interfaces of two layers, resulting in a alloy layer only few monoatomic layers thick. This interface roughness can only be seen in a thick superlattice if the substrate is doped so it tends to have a metallic behavior, with the reflectivity coefficient at the buffer–substrate interface approaching to 1 [7]. In our case the substrate is not doped but the buffer layer has a negative ϵ in a much wider region than the superlattice so it acts as a mirror in the AlAs "Reststralen" region. Here the radiation is reflected back and passed again through the SL. As a result the reflectivity spectrum includes features peculiar of transmission through a film of double thickness [8].

In fig.4 we show the influence of the buffer layer on the FIR spectra. As can be seen the influence is week in the "Reststhralen" regions, for both the GaAs and AlAs regions, but is significant between these to regions. This is due to high absorption in these two regions. The influence of the buffer layer extend as far as the low energy side of th AlAs "Reststhralen" region, almost up to the ω_{TO} of the AlAs like phonon frequency of the $Al_xGa_{1-x}As$ from the superlattice.

5 Conclusion

We have presented infrared experimental spectra, at normal incidence angle and at room temperature of a thick $GaAs/Al_xGa_{1-x}As$ superlattice with a 0.5 μm buffer layer. We had then used a standard iterative procedure to calculate the spectra and from the ensuing fit we obtained the values of optical and structural parameters of the constituent layers. The structural parameters include the layer thicknesses and the optical parameters, the phonon frequencies, damping constants, oscillator strengths and dielectric permitivities. The fitted parameters, both structural and optical, are in a very good agreement with the values obtained elsewhere [6]. The necessity to include the buffer layer during the calculation of the spectra is shown and the thickness of the buffer layer is determined with a good accuracy, although the buffer layer is deeply burried beneath the 7.6 μm SL. For the first time the influence of the buffer layer, which is located deeply below the structure of a superlattice, on the reflectivity spectrum, has been numericaly analized using an iterative model.

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Refleksioni infracrveni speltri debele superrešetke sa medjuslojem

Abstrakt: U ovom radu ispitivani su spektri GaAs/AlGaAs debele superrešetke sa medjuslojem u dalekoj infracrvenoj oblasti do 450 cm^{-1}. Uočen je veliki uticaj medjusloja na refleksione spektre u transparentnim delovima, izvan "Reststrahlen" oblasti GaAs i AlAs. Pokazano je da se jednostavnom iterativnom metodom, u aproksimaciji efektivnog medijuma, mogu vrlo tačno odrediti strukturni parametri ne samo superrešetke već i medjusloja.

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