STRUCTURAL ANALYSIS OF THE $Al_xGa_{1-x}As/GaAs$ MULTI QUANTUM WELL STRUCTURE

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Molekulyar Şüa Epitaksiyası (MBE) metodu ilə çoxlu kvant quyulu (MQW) $Al_xGa_{1-x}As/GaAs$ strukturlar alınmışdır. Şürüşən düşmə bucağı ilə Reflektrometirya və yüksək həssasiyətli Rentgen difraksiyası (HRXRD) ilə ölçülərdən alınmış nəticələrə əsaslanaraq alınmış strukturların kristal quruluş parametrləri verilmişdir. Alttaşdan (002) istiqamətində simmetrik əsaslanmadan alınmış struktur parametrləri LEPTOS proqramı vasitəsi iə dinamik və kinematik yanaşma çərçivəsində modelləmə yolu ilə təsdiq edilmişdir.

Методом молекулярной лучевой эпитаксии (МЛЭ) поучены $Al_xGa_{1-x}As/GaAs$ структуры с мульти квантовыми ямами (МКЯ). На основе данных рефлектометрии при скользящем угле падения, рентгеновской дифракцией высокого разрешении (HRXRD) и рентгеновского распределения сигнала в обратном пространстве, сообщаются структурные параметры полученных структур. Данные по кривым качания и отражения полученные при измерении симметричного отражения от подложки в направлении (002) были подтверждены моделированием с использованием программы LEPTOS в рамках динамического и кинематического подхода.

In this work a $Al_xGa_{1-x}As/GaAs$ multi quantum well (MQW) structure has been grown with solid source molecular beam epitaxy (MBE) system. Structural parameters for the MQW structure were reported by using grazing incidence reflectometry, high-resolution X-ray diffraction (HRXRD) and reciprocal space mapping. The Rocking and reflectivity scans were measured by HRXRD system on (002) symmetric reflection of substrate has been simulated using LEPTOS program within the framework of dynamic and kinematical theories.

1. INTRODUCTION

Multi quantum well structures (MQW) are attractive material systems in the development of the electronic devices in modern technology. The Schottky diodes, field effect transistors (FET) and the injection lasers are prepared from GaAs and AlGaAs based nanodimensional heterostructures [1,2,3]. Currently in the producing of nanodimensional multi quantum wells and quantum dots, molecular beam epitaxy (MBE) is used rather than other growth techniques[4,5,6]. These low dimensional structures show unique physical properties, particularly interesting for novel optoelectronic devices like QD lasers with a higher differential gain and a lower threshold current density [7].

In spite of the tremendous interest in self-organized quantum well structures there is only scarce information available on the crystallographic properties and their strain states. For this purpose, transmission electron microscopy (TEM) [8], atomic force microscopy and scanning tunneling microscopy (STM) [9] have been used, even with atomic resolution [10]. However, these techniques are either destructive or they cannot be used for samples grown with cap layers.

During the last 20 years interest in high-resolution X-ray diffractometry and reciprocal map has grown as a result of the development of the semiconductor industry and the increasing interest in material research of the various thin layers. HRXRD allows the evaluation of interface thickness, concentration, strain and relaxation of epitaxial heterostructures. The reciprocal space is an alternative detailed representation of the crystal system [11].

Grazing incidence X-ray scattering methods play a key role in the characterization of the surface region by controlled the penetration depth. Among these grazing incidence techniques, X-ray reflectometry, has been shown to be a well-suited tool to assess structural details of low-dimensional systems on length scales from several Angstroms to hundreds of nanometers. X-ray reflectivity provides a wealth of information on thickness and interfacial properties on the nanometer scale, such as layer thickness, the layer‘s electronic densities, surface and interface roughness and roughness morphology. The reflectometry method is, therefore, well suited for the study of surfaces and thin layers. It provides several important advantages: the physics beyond is quite simple, the experiments are relatively simple to perform, X-ray techniques are highly developed, it is a non-destructive technique (except upon biological samples), measurements are possible in various temperatures, humidities, pressures, etc.[12].

In this paper, a comprehensive X-ray analysis of $20x(Al_xGa_{1-x}As/GaAs)$MQWs grown by MBE is presented. The x-ray diffraction and reciprocal space mapping measurements were performed by D8-Discover diffractomer equipped on the primary side with a Ge(220) monochromator and a horizontal divergence slit with a width of 1mm. On the secondary side, the reflected light passes a horizontal slit with a width of 0.1mm before entering the wide open scintillation detector.

2. EXPERIMENTAL PROCEDURE

Sample was grown on epi-ready p-type GaAs (100) substrate by molecular beam epitaxy using a VG-Semicon V80H solid source MBE system. Arsenic was supplied in the form of As_2 from a valved cracker cell and its beam equivalent pressure was $1.0x10^{-5}$ mbar. The substrate was outgassed at 400 ^oC for two hours in preparation chamber before oxide desorption was performed by heating up to 590

^oC with As_2 flux irradiation in the growth chamber. At this stage, surface structure was checked by RHEED pattern observation. After fully oxide desorption, first, a 0.5 μm undoped GaAs buffer layer on the substrate was grown with 2.78 Å/s growth rate at 580 substrate temperature. Secondly a MQW (20 repeats) period is compose of two layer. The first layer is undoped 150Å $Al_{0.2}Ga_{0.8}As$ layer was grown with 0.44 Å/s growth rate for AlAs and 1.67 Å/s growth rate for GaAs. The second, undoped 50Å GaAs layer was grown with 1.67 Å/s growth rate. The sample structure is given in Fig. 1. during the growth process deposition chamber pressure was $5.2x10^{-7}$ mbar.

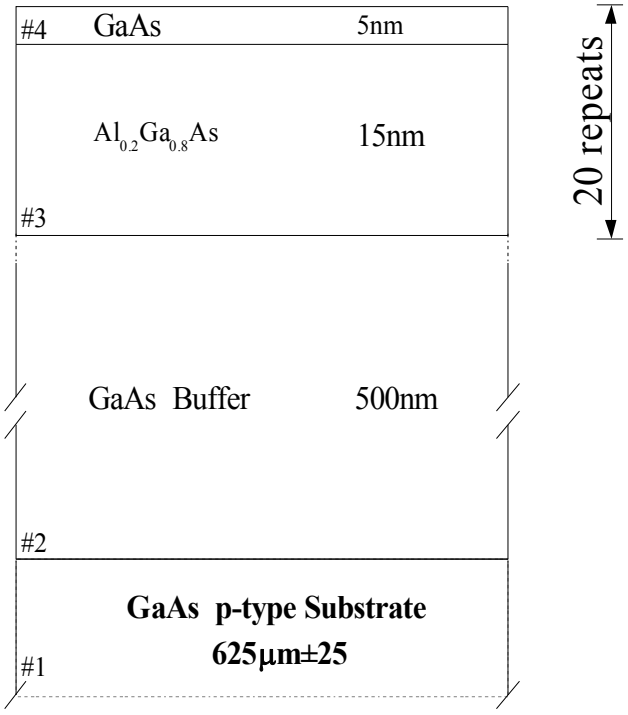

Fig. 1. $Al_{0,2}Ga_{0,8}As$/GaAs MQW structure with nominal values of the layer thicknesses and Al concentration.

For the high resolution X-ray measurements (HRXRD), have been used a five-crystal diffractometer built at the Bruker-AXS, GmbH, Karlsruhe. Originally, the instrument was designed to measure the atomic form factors of perfect volume crystals. For this purpose an extremely high angular resolution of 12inc (0.0033^o) is reached by applying a torque on a lever arm which is connected with the goniometer axis. For the investigation of heteroepitaxial samples described here the sample stage was mounted a goniometer. The monochromating unit consists of a four-reflections channel-cut (220) oriented Ge crystal in the (+n, -n, -n, +n) mode as a beam conditioner. With this setting, the rocking curves widths smaller than 5 arcseconds have been measured for the Si(004) and sapphire (0006) reflections. The X-ray diffraction measurements were performed with a fixed Cu anode ($CuK_{\alpha 1}$, $\lambda = 1.5406A$) at 2.2 kW.

3. RESULTS AND DISCUSSION

ω-2θ X-ray reflectivity scan for the azimuthal orientation of the sample were performed using $CuK\alpha$ radiation as shown in Fig. 2. In principle, the thicknesses of the layers, their chemical composition as well as the root mean square roughness (rms) of the interfaces can be obtained from such measurements. As shown in the figure 3, the plateau region in the about $0-0.7^0$ interval is strongly smooth which suggests that sample surface is uniform. The measured specular reflection curves exhibit periodical satellite maxima; their height is influenced by the interface roughness and by the thickness of the individual layers building up the multilayer period. Surprisingly, depending on the direction of the incidence of the X-ray beam, the maxima are modulated by a position-dependent envelope function [12]. There is a more or less pronounced symmetric shoulder associated with each maximum indicating highly symmetric interfaces. In addition there is a strong contribution of a background which also depends on the sample orientation. After subtracting a diffuse background, a best fit is obtained with a thickness of $15.6219 \pm 0.1\%$ nm for the (Al,Ga)As layers with a rms roughness of σ =1.99640 $\pm$ 0.1 nm and $4.8578 \pm 0.1\%$ nm for the GaAs layers with a rms roughness of σ = 1.22610 $\pm$ 0.1 nm.

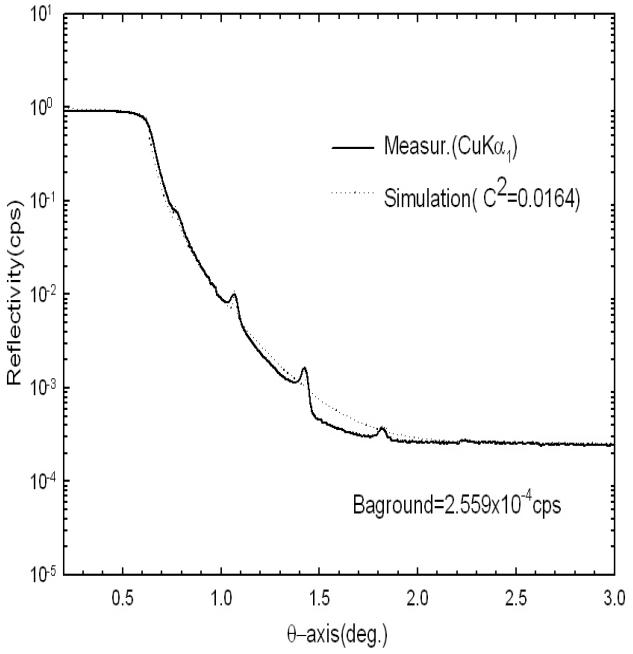

Fig. 2. Specular reflectivity of 20x MQW Solid line shows experimental data and dotted line gives fit curve.

Reflectivity measurements were simulated by LEPTOS program which is supported by Simulated annealing method [13]. This is a global optimization method derived from Monte Carlo methods. As shown in Fig.2, the reflectivity exhibits fringes (Kiessig fringes) which are related to the layer thickness. The reflection of X-rays can be treated with a kinematical approximation just like in reflection of visible light, with the reflection /transmission being described by the well-known Fresnel equations.

In Fig. 3, we have plotted conventional high resolution five crystal rocking curves obtained with $CuK\alpha_1$ radiation for the symmetrical (002) Bragg reflection with k along the [110] direction. In this figure, the simulation of HXRD scan using the computer program [13] based on the solution of the Takagi-Taupin equations of dynamical diffraction theory is also given [14]. As shown in the figure, two different diffractions in the middle and near to edge of the wafer are taken. These curves give similar results and the parameters

calculated from each diffraction pattern are averaged.

The position of the sample was adjusted in order to provide maximum intensity from the substrate peak. Good agreement between experiment and simulation is obtained with a layer sequence of 20x (4.8578nm GaAs, 15.6219nm $Al_{0.2}Ga_{0.8}As$, placed on 544.8304 nm GaAs buffer) assuming a good tetragonally distorted layer system. Because, in strain analysis, dc/c Top/Bot which are the normal (perpendicular to the sample surface) lattice mismatches are obtained from simulation as $3.551x10^{-08}$ and $1.003x10^{-03}$ respectively. This value shows clearly that at increasing periods to perpendicular to surface, the strain structure has shifted weakly to relaxation status. It should be noted that the symmetrical (002) reflection is only sensitive to the lattice strain perpendicular to the layers. The obtained values from HXRD measurements are collected to compare with XRR in Table 1. It concludes that there is a perfect agreement between every two measurements.

Table 1. Simulation results obtained from XRR and HXRD.

Layer	ρ_{sim} $\pm0.03 g/cm^2$	$\rho_{theo.}$ g/cm^2	*t(nm)* ±1%		σ(nm) ±0.1	X
	XRR	-	XRR	HXRD	XRR	HXRD
#4	5.6338	5.3176	4.8578	4.856	1.2261	-
#3	5.4846	4.9889	15.622	15.621	1.9964	20.7
#2	5.2527	5.3176	544.83	544.829	4.1530	-

The angular position of the 1th order quantum well peak was determined calculating the mean Aluminum content in the whole multi quantum well system in the growth direction, which is 20.7%. On the left hand side of the substrate peak, multi quantum well satellite peaks up to the order -4 are visible. On the right hand side, the multi quantum well peaks +1 to +4 can be observed. The disappearance of the multi quantum well peak is due to destructive interference effects depending critically on the individual layer thicknesses. We obtained excellent agreement with the reflectivity measurements.

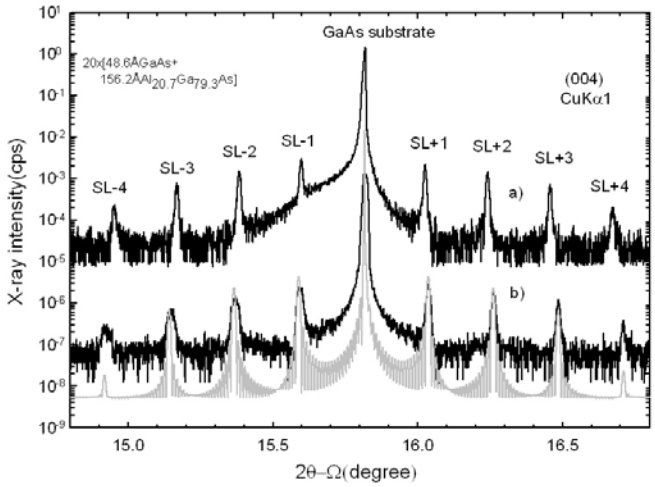

Fig. 3. High-resolution Bragg reflection in the vicinity of the (002) reflection of 20x multi quantum well stack. Reflections given in a and b labeled plots were measured from different two point of wafer in order to observe well the layer peak. Gray line shows the simulation curve.

The (004) quantum well peaks show an asymmetric splitting which increases with increasing order and produces an asymmetric shape for the higher-order satellite peaks. We tried to simulate this effect by a gradient in the Aluminum concentration in the growth direction [15]. However, the thickness of the Al-containing layers is very thin to determine the asymmetry in the present quantum wells. As has been pointed out in ref. [16] all random-type interfaces would cause a broadening of the diffraction lines leaving their position unaltered. Such a broadening is not observed here.

The reciprocal map for a (002) diffraction of the (Al, Ga)As quantum well structure is shown in Fig. 4 The intensity maxima of the GaAs- buffer layer and the MQW system is set along the line $\omega = \theta$, indicating that the MQW is uniform with respect to the GaAs-buffer layer. This result is in consistent with the reflectivity result. Along the ω-2θ-direction ($q_{\perp}$-direction), stain variation and thickness fluctuations of the SL can be seen clearly along the growth direction in the figure. In the ω-direction ($q_{//}$), it is apparent that the structure peaks exhibits some mosaic spread which increases considerable for the higher SL satellites. In addition, an analyzer streak isn't also observed in the angular direction. As seen in high-resolution Bragg reflection, in the fig. 4, SL satellites are visible clearly and all peaks were labeled. In right upper field of the figure, the larger scan for the substrate has been taken, and from this figure it can be seen that all peaks due to substrate peak lies on a large scale along (110) azimuth orientation of the sample.

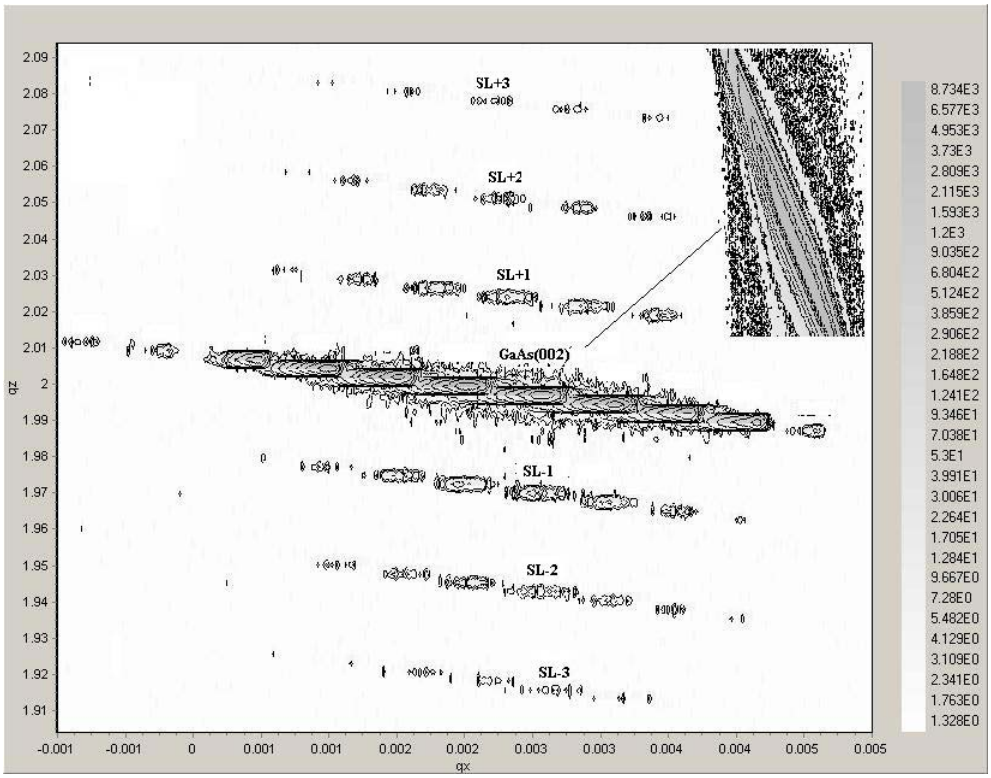

Fig. 4. Reciprocal space maps measured on an (Al,Ga)As multi quantum well

4. CONCLUSION

A 20 fold AlGaAs/GaAs multi quantum well structure was grown by solid source MBE system. The structural properties of the MQW were investigated by different X-ray methods in detail. From X-ray reflectivity measurements have been obtained the interface roughness and the thickness agreed well with its nominal values for the individual layers. From high-resolution measurements a weak tetragonally distorted superlattice structure is found with a mean Al-concentration of 20.7% in the (Al,Ga)As/GaAs structure. Results obtained from every two measurement are in the perfect agreement. As last analysis, the reciprocal map of multi quantum well structure was researched.

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