

AKÜ FEMÜBİD 20 (2020) 041101 (558-564)

AKU J. Sci. Eng. 20 (2020) 041101 (558-564)

DOI: 10.35414/ akufemubid.707628

Araştırma Makalesi / Research Article

Characterization of GaAs/GaAlAs Heterostructures Grown on GaAs Substrate using High Resolution X-ray Diffraction Method

Habibe SAYRAÇ^{1,2*}, Muhammed SAYRAÇ³, Sezai ELAGÖZ⁴¹Department of Physics, Faculty of Science, Gazi University, 06500 Ankara, Turkey.²Vocational School of Health Services, Ankara Medipol University, 06050 Ankara, Turkey.³Department of Physics, Faculty of Science, Cankiri Karatekin University, 18100 Cankiri, Turkey.⁴AELSAN-Microelectronics, Guidance & Electro-Optics, Ankara, Turkey.

Sorumlu yazar e-posta: habibe.sayrac@gazi.edu.tr

ORCID ID: <http://orcid.org/0000-0002-4566-7736>

muhammedsayrac@karatekin.edu.tr

ORCID ID: <https://orcid.org/0000-0003-4373-6897>

elagoz@cumhuriyet.edu.tr

ORCID ID: <https://orcid.org/0000-0002-3600-8640>

Geliş Tarihi: 23.03.2020

Kabul Tarihi: 21.08.2020

Abstract

Characterization of nanostructures using X-ray diffraction (XRD) method gives information on the composition, the lattice strain, and heteroepitaxial layers of the structures. These information are useful for fabrication process of optoelectronic devices. In this paper, we give fundamental description to the commonly used material, GaAlAs. In addition, the importance of X ray diffraction method for characterization of the materials provides crucial information for the growth and development process of the materials. Structural characterization of epitaxial growth GaAs/GaAlAs heterostructures are analyzed using the X- ray diffraction (XRD) method. Rigaku Global Fit simulation program is performed to compare the experimental results, and the simulation and the experimental results agree with each other.

Keywords

GaAs; GaAs/GaAlAs;
XRD; MBE; Epitaxial
Growth

GaAs Alttaş Üzerine Büyütülen GaAs/GaAlAs Heteroyapılarının Yüksek Çözünürlüklü X- Işını Kırınım Yöntemi Kullanılarak Karakterizasyonu

Öz

Nano yapıların X- ışını kırınımı (XRD) yöntemi kullanılarak karakterizasyonu, bu yapıların bileşimi, örgü zorlanması ve heteroepitaksiyel katmanları hakkında bilgi verir. Bu bilgiler optoelektronik cihazların üretiminde önemli rol oynamaktadır. Bu makalede, yaygın olarak kullanılan GaAlAs malzemesi hakkında genel bilgilerden bahsedilmektedir. Ek olarak, X- ışını kırınım yönteminin malzemelerin karakterizasyonu için önemi, malzemelerin büyüme ve yapının oluşum süreci hakkında önemli bilgiler sağlamasıdır. Epitaksiyel olarak büyütülmüş GaAs/GaAlAs heteroyapılarının yapısal karakterizasyonu X- ışını kırınım yöntemi kullanılarak analiz edilmiştir. Deneysel sonuçları karşılaştırmak için Rigaku Global Fit simülasyon programı kullanıldı, simülasyon ile deneysel sonuçların yüksek oranda uyumlu olduğu görüldü.

Anahtar Kelimeler

GaAs; GaAs/GaAlAs;
XRD; MBE; Epitaksiyel
Büyütme

© Afyon Kocatepe Üniversitesi

1. Introduction

GaAlAs materials have been well known for their suitability for optical devices, for example, solar cells, laser diodes and light emitting diodes because of their band gap structure and high mobility (Liu et al. 2012, Kish et al. 1991, Kato et al. 1991, Neamen 2003). The promise of these devices has led to numerous studies to obtain more effective structures using progressive growth

systems (Thompson 1997, Liu et al. 2004). GaAs substrate has absorbing properties Schubert (2006), however, it has been preferred for fabricating optical device based on GaAlAs material because of that GaAs is lattice matched with GaAlAs material (Schubert 2006).

Ga and As are elements from groups III and V in the periodic table and are direct band gap semiconductors. Electrons emitting or absorbing

photons travel between the valance and the conduction band. These materials can be used in diode lasers, and the emitted wavelength is determined from the band gap of the material. The sophisticated growth techniques make possible a crystal perfectly grown using a mixture from groups III and V elements. Mixture of GaAs with AlAs gives

AlGaAs ternary compound, which has useful features. The band gap of GaAs is different from that of AlAs. The band gap value can be chosen by controlling the proportions of Ga and Al in the compound. Thus, the emitted wavelength by the laser can be tuned that results important applications on laser based devices (Hayashi and Marcon 2000).

X-ray diffraction systems are used to determine the characteristic structural parameters of artificial semiconductor-based super lattices (Horikoshi et al. 1986, Auvray et al. 1987). The growth of a structure requires very high precision methods such as metalorganic chemical vapor deposition (MOCVD) or molecular beam epitaxy (MBE) system. The growth process needs to be checked whether the structure is growth the way it is supposed to be. The control of the crystal structure is performed by using X-Ray Diffraction (XRD) method. The structural feature obtained by the epitaxial growth process is necessary to know for researchers working on nano heterostructures.

In this paper, we aim to analyze structural characterization of epitaxial growth GaAs/GaAlAs heterostructures using the X- ray diffraction (XRD) method. In addition, the simulation of XRD data is performed by Rigaku Global Fit simulation program. The experimental and the computational results are compared, and they are in close agreement. Even though there are many researches have been completed using XRD method, it is important to find best structural properties of the nanostructure.

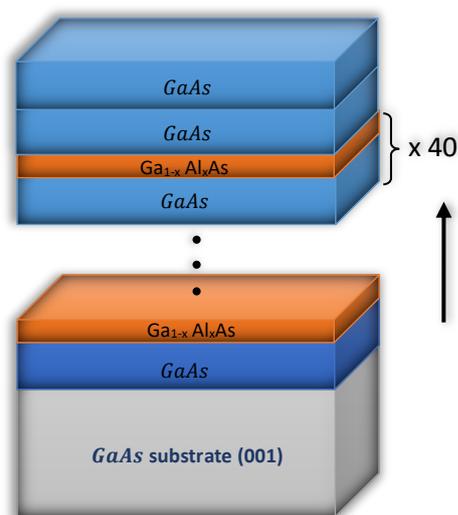


Figure 1. Schematic demonstration of the GaAs/Ga_{1-x}Al_xAs heterostructure.

2. Experimental

The GaAlAs structure were grown on a GaAs substrate using molecular beam epitaxy (MBE) system. The Figure 1 presents demonstration of GaAs/ Ga_{1-x}Al_xAs superlattice structure, which four different alloy ratios of each repeated 10 times growth by MBE crystal growth technique, on the (001) crystal oriented GaAs substrate. The nanostructures obtained by epitaxial crystal growth methods are subsequently obtained by using various lithography techniques. The epitaxial crystal growth is based on the growth parameters, which directly affect the crystal quality such as uniformity and crystal thickness. These parameters directly affect the structural, electrical, and optical properties of the crystal.

The crystallization and growth direction for the GaAlAs structure grown on GaAs substrate were measured by using the θ -2 θ scan, ω scan, and Φ scan. The experimental results are compared with the simulation results which are in agreement with each other.

3. Results and Discussion

Rigaku SmartLab X-ray diffractometer is used to analyze the structural properties of the growth structure. The device performs structural analysis of thin films, dust and bulk samples. To generate the X-ray source, copper (Cu) target with rotating

anode is used. The wavelength of X-rays is $K_{\alpha 1} = 0.154059$ nm, and its power is 9 kW (max voltage 45 kV, max current 200mA).

The X-ray diffraction analysis comes from fundamental the Bragg law (Ashcroft and Mermin 1976)

$$n\lambda = 2d \sin \theta \quad (1)$$

here n is a positive integer, λ is the wavelength of the source used for characterization, θ is the angle between incident ray and the scatter plane, and d is the spacing of the crystal layers (Quinn and Yi 2009).

The relationship between the spacing of the layers and the lattice constant for cubic crystal structure are given law (Ashcroft and Mermin 1976)

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (2)$$

where d is the spacing of the crystal layers, a is the lattice constant and h, k, l are Miller indices (Pahuja 2005). By using the experimental result, information about the structure of thin multi-layer structure such as lattice constant, stacking, crystal structure, roughness, lateral coherence length, change of layer thickness, sharpness of interfaces, diffusion between layers, vertical stress and crystallographic orientation of materials are obtained from X-ray diffraction pattern. The experimental results could be compared well known Bragg formula, Eq. 1 and Eq. 2.

The experimental results are characterized using four different scan methods to understand and to investigate the properties of the structure. These scans, which are briefly described in below are important to understand the features of the GaAlAs structure.

4. X Ray Diffraction

4.1 θ - 2θ scans

The θ - 2θ scans are usually created in reflection geometry and sometimes is called as (001) scans. These radial scans allow us to scan sample planes parallel to the growth direction. In θ - 2θ scans, not only the substrate peak but also the superlattice peaks are clearly observed. The intensity of the peaks decrease from the center to the outside, and the first four satellite peaks are a clear indication that the quality of the growth process is quite good.

The difference between the theoretical and experimental lattice constant of the GaAs substrate is calculated from wide angle scans. Bragg angle for GaAs (004) was taken from the Fig. 2. Miller indices ($h=0, k=0, l=4$) and the Bragg angle are written in Eq. 1 and Eq. 2. Then the lattice constant for GaAs was found $a_{GaAs} = 5.6539\text{\AA}$, and it is in agreement with the literature ($a_{GaAs} = 5.65325\text{\AA}$) (Börnstein 1999). The relative error between the values in the literature and the calculation is 0.011%.

Figure 2 shows the scan of GaAs/Ga_{1-x}Al_xAs structure from (a) 30.5° to 33°, and (b) 65.7°–66.5°. The peaks are sharp, and intensities of the peaks are decreasing from the center to the edge. These peaks are called satellite peaks, and it is a clear indication that the quality of the growth is quite good.

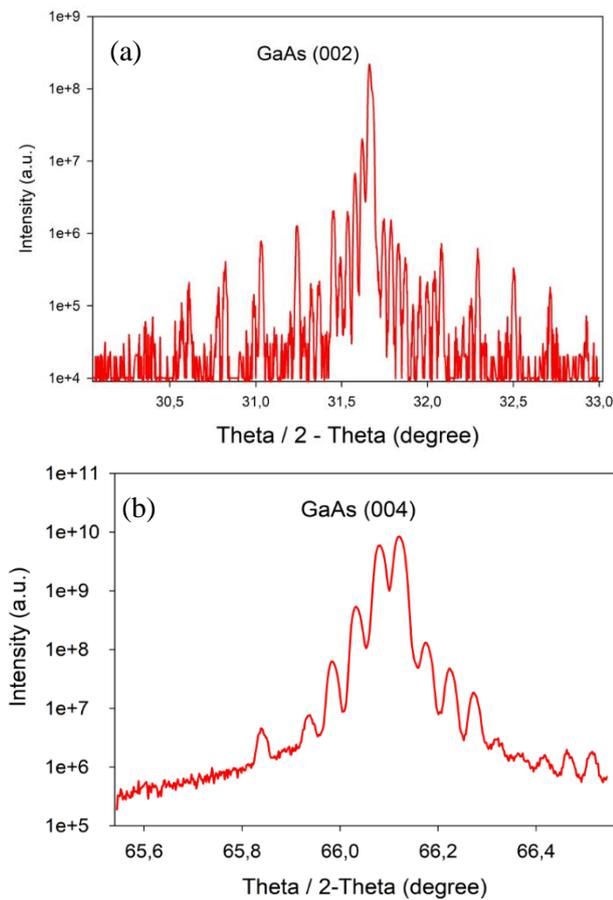


Figure 2. High-resolution θ - 2θ scan of GaAs/Ga_{1-x}Al_xAs heterostructure. 2θ scan is between (a) 30.5°–33°, and (b) 65.7°–66.5°.

4.2 Rocking curve scan (ω scan)

Rocking curve scan (ω scan) provides information about the roughness of the structure interfaces and the lateral coherence length. Figure 3 shows the ω scan for GaAs/Ga_{1-x}Al_xAs heterostructure on (004) plane. As a result of the GaAs peak, the full width half maximum (FWHM) was calculated 0.01°, and the lateral coherence length was found 1611 nm. In plane scan and phi scan need to be performed for controlling the epitaxial growth, but the structure thickness is not suitable to perform in plane scan. The structure could be thinned for scanning, however it is not required since asymmetric scan gives the similar results.

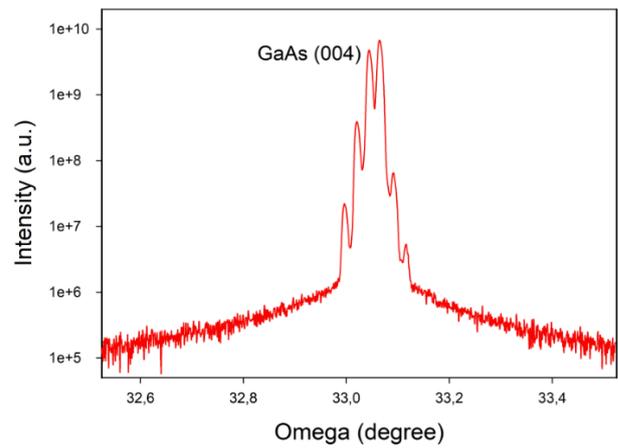


Figure 3. ω scan for GaAs/Ga_{1-x}Al_xAs heterostructure (004) peak.

4.3 Asymmetric Scan

The lattice constant of the GaAs crystal is calculated, and lattice constant for GaAs (202) plane is found $a_{GaAs}=5.6554 \text{ \AA}$. Bragg angle is experimentally estimated from Figure 4, and the theoretical Miller indices ($h=2, k=0, l=2$) for GaAs (202) is calculated from Eq. 1 and Eq.2. The error

$$\left(\frac{|a_{\text{experiment}} - a_{\text{theory}}|}{a_{\text{theory}}} \times 100 \right) \text{ is estimated } \sim 0.038\%$$

compared to the lattice constant of GaAs in the literature ($a_{GaAs} = 5.65325 \text{ \AA}$) [14]. The lattice constants are calculated using the results of symmetric and asymmetric scans, and they are very close to each other and the literature value Börnstein (1999), showing that the growth is achieved in harmony.

An important control of epitaxial crystal growth is that in-plane peak positions of the sample and the substrate are the same. Figure 4 shows that θ - 2θ scan of GaAs/Ga_{1-x}Al_xAs structure between 44.8°–45.8° on (202) plane.

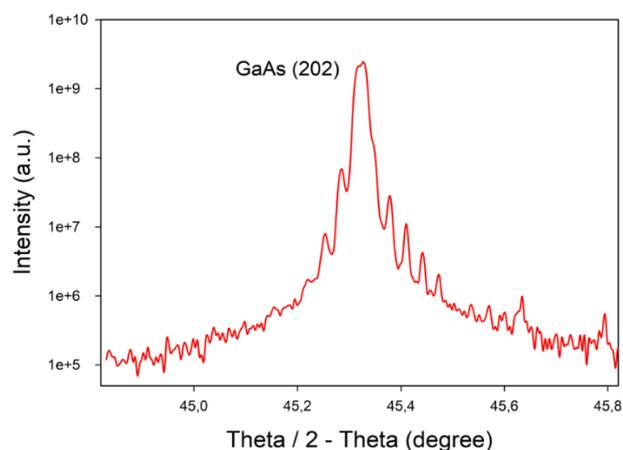


Figure 4. θ - 2θ scan for GaAs/Ga_{1-x}Al_xAs structure between 44.8°–45.8° on (202) plane.

4.4 Φ Scan

Phi (Φ) scan gives the investigation about the perpendicularity of the surface, curvature of the substrate, and the surface in-out plane geometry. Figure 5 shows the pattern of refraction is repetitive in every 90°. It means that the GaAs crystal has a cubic structure, and the epitaxial growth occurs. The Rigaku SmartLab X-ray diffractometer used in the asymmetrical Φ scan produces the same as intensity of the peaks (Fig. 5), and it can be concluded that the epitaxial growth of heterostructure is reasonable.

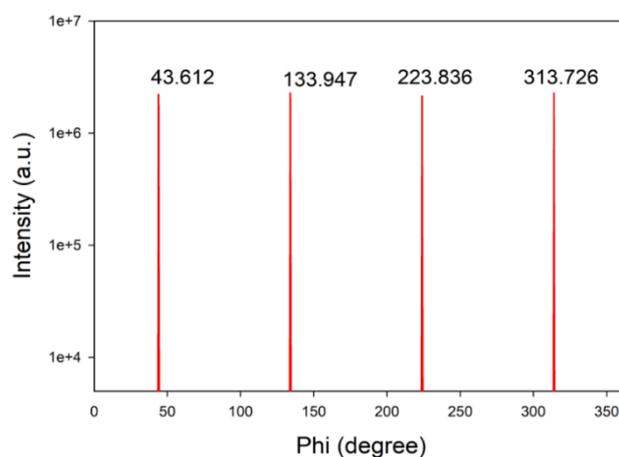


Figure 5. Φ scan for GaAs/Ga_{1-x}Al_xAs heterostructure between 0°–360°.

5. Simulation

Simulation for GaAs/Ga_{1-x}Al_xAs heterostructure is performed using the Rigaku GlobalFit simulation software program. The simulation program for (002) and (004) GaAs peaks are applied, and

simulation is performed for controlled parameters such as thicknesses and doping ratio. With the changing in the doping percentages for the Ga_{1-x}Al_xAs layers, the simulation better overlaps to the experiment, Figure 6. The simulation results are compared with the experimental results. The Figure 6 shows that simulation of the (002) peak for GaAs/Ga_{1-x}Al_xAs heterostructure.

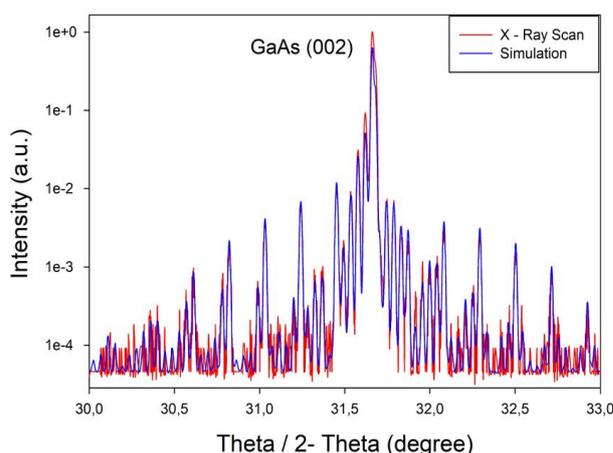


Figure 6. Simulation and experimental graphics for GaAs/Ga_{1-x}Al_xAs (002) peak. Red line is X-ray scan from Fig. 2 (a), and the blue line is the simulation results.

Figure 7 is that the simulation and the experimental plot of the (004) peak of GaAs/Ga_{1-x}Al_xAs heterostructure are performed for the angle between 65.7°–66.5°. It shows that the experimental and simulation results are in agreement with Figure 2 (b). Intensities of the peaks are normalized to unity for better comparison in Figure 6 and 7.

Optimum parameters giving best fit to experimental results are obtained, and they are presented in Table 1, which gives information about (002) and (004) peaks. The layer thickness, the doping rates and their averages are compared. Although there are not many differences between layers thicknesses in theoretical and experimental (Average Layer Thickness) values, alloy ratios are relatively different. This difference in alloy ratios determines the efficiency of the device, and they are directly linked to the quality of the devices.

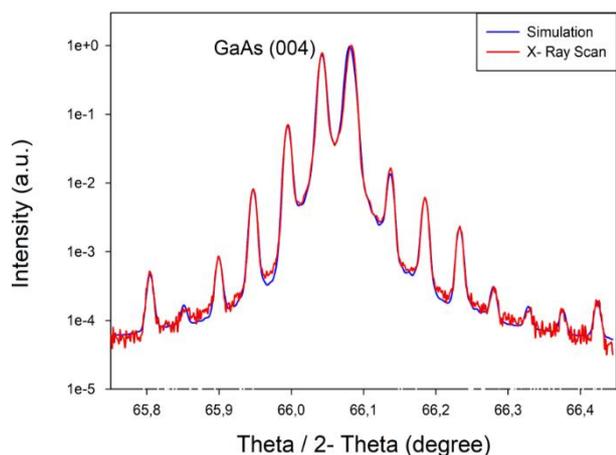


Figure 7. Simulation and experimental graphics for GaAs/Ga_{1-x}Al_xAs (004) peak. Red line is X-ray scan from Fig. 2 (b), and the blue line is the simulation results.

The GaAs/Ga_{1-x}Al_xAs heterostructure is a cubic structure because of the repetition of the peaks every 90°, Fig. 5. It has been shown that the uniformity of the crystals is good because the yields of the peaks are equally spaced, Fig 5. This underlines the fact that the X-ray diffraction method is indeed an important method of characterization, and it is an initial analyzing state to see the growth method is achieved the way it is expected before going other characterizations stage.

Table 1. Compare of the simulation and theoretical parameters for GaAs/Ga_{1-x}Al_xAs heterostructures (002) and (004) peak.

Layer	Theoretical		Experimental Growth Structure				Average Doping Rate of 002 and 004 (%)	Average Layer Thickness of 002 and 004 (nm)
	Doping Rate (%)	Layer Thickness (nm)	(002)		(004)			
			Doping Rate (%)	Layer Thickness (nm)	Doping Rate (%)	Layer Thickness (nm)		
GaAs		1000		1162		1054	1108	
GaAs		50		49.8		49.5	49.6	
Ga _{1-x} Al _x As	21.0	40	31	37.3	26.5	38.2	29	37.7
GaAs		5.5		6.4		6.2	6.3	
Ga _{1-x} Al _x As	24.0	40	22.1	36.8	21	42	21.5	39.4
GaAs		5		6.4		3.6	5	
Ga _{1-x} Al _x As	30.0	40	40	37.5	42	35	41	36.3
GaAs		4		5.2		2	3.6	
Ga _{1-x} Al _x As	35.0	40	30	38.8	26.8	45	28.5	41.8
GaAs		1500		375		750	562.5	
GaAs (substrate)		Infinite		Infinite		Infinite	Infinite	

6. Conclusion

In this paper, (001) crystal-oriented GaAs on the bottom of the epitaxial growth four different alloy ratios of each repeated 10 times GaAs/Ga_{1-x}Al_xAs

superlattice structure growth by MBE crystal growth technique was studied, Fig. 1. During the structural analysis, Rigaku SmartLab ultra-high resolution X-ray diffraction system was used. The

GaAs/Ga_{1-x}Al_xAs structure was studied using θ -2 θ scan, ω scan, and Φ scan.

The structural characterization of GaAs/Ga_{1-x}Al_xAs structure growth on GaAs substrate by MBE technique is analyzed by using XRD technique. The simulation is performed to compare to experimental results. They are in agreement with the experimental results. The presented work is important to find and to determine the structural properties of the nano structure, and it is first step whether the structure is growth the way it is expected. This works gives brief introduction of the XRD method on the scientific and engineering method. The improved result can find in application areas from light emitting diode (LED) to scientific instrument.

7. References

- Ashcroft N. W. and Mermin N. D., 1976. Solid State Physics, **116**, Saunders College Publishing, Orlando, 217.
- Auvray P., Baudet M. and Regreny A., 1987. X-ray diffraction study of intentionally disordered GaAlAs-GaAs superlattices. *Journal of Applied Physics*, **62**, 456-460.
- Börnstein L., 1999. Semiconductors II-VI and I-VII Compounds; Semimagnetic Compounds, *Springer Materials*, **41B**.
- Hayashi M. and Marcon R., 2000. High Resolution X-ray diffraction to characterize semiconductor materials. *Physica*, **1**, 21-27.
- Horikoshi Y., Kawashima M. and Yamaguchi H., 1986. Low-temperature growth of GaAs and AlAs-GaAs quantum-well layers by modified molecular beam epitaxy. *Japanese Journal of Applied Physics*, **25**, L868-L870.
- Kato T., Susawa H., Hirotani M., Saka T., Ohashi Y., Shichi E. and Shibata S., 1991. GaAs/GaAlAs surface emitting IR LED with Bragg reflector grown by MOCVD. *Journal of Crystal Growth*, **107**, 832-835.
- Kish F. A., Caracci S. J., N. H. Jr., Dallesasse J. M., Höfler G. E., Burnham R. D. and Smith S. C., 1991. Low-threshold disorder-defined native-oxide delineated buried-heterostructure Al_xGa_{1-x}As-GaAs quantum well lasers. *Applied Physics Letters*, **58**, 1765-1767.
- Liu C. Y., Yuan S., Dong J. R. and Chua S. J., 2004. Temperature dependence of photoluminescence intensity from AlGaInP/GaInP multi-quantum well laser structures. *Journal of Crystal Growth*, **268**, 426-431.
- Liu X. Q., Fetzer C. M., Rehder E., Cotal H., Mesropian S., Law D. and King R. R., 2012. Organometallic vapor phase epitaxy growth of upright metamorphic multijunction solar cells. *Journal of Crystal Growth*, **352**, 186-189.
- Neamen D. A., 2003. Semiconductor Physics and Devices, **4**, Avenue of the Americas, 17-19.
- Pahuja O. P. Dr., 2005. Solid State Physics, **1**, SP/Laxmi Publications, New Delhi, 45-47.
- Quinn J. J. and Yi K.-S., 2009. Solid State Physics Principles and Modern Applications, **2009**. Springer, 3-36.
- Schubert E. F., 2006. Light-Emitting Diodes, **2**. Cambridge University Press, Edingburgh Building, 86-100.
- Thompson A. G., 1997. MOCVD technology for semiconductors. *Materials Letters*, **30**, 255-263.