The Rigaku Journal
Vol. 14/ number 2/ 1997

CONTRIBUTED PAPERS

X-RAY DIFFRACTION ANALYSIS OF SELF-ORGANIZED InAs QUANTUM DOTS IN MBE GaAs/InAs/GaAs (001) SANDWICH STRUCTURE

Y. ZHUANG, Y.T. WANG, W.Q. MA, W. WANG
National Research Center for Opto-electronic Technology, Institute of Semiconductor, Chinese Academy of Science, P.O. Box 912, Beijing 100083, China

X.P. YANG, Z.Q. CHEN, D.S. JIANG, H.Z. ZHENG
Beijing Laboratory of Superlattice and Microstructures, Institute of Semiconductor, Chinese Academy of Science, P.O. Box 912, Beijing 100083, China

A series sample of GaAs/InAs/GaAs were studied by double crystal X-ray diffraction and the X-ray dynamic theory were used to analyze the X-ray diffraction results. As the thickness of InAs layer exceeded 1.7 monolayer, 3-dimensional InAs islands were occurred. Pendellosung fringes were shifted. A multilayer structure model is proposed to describe the strain status in the InAs islands in the sample and a good agreement obtained between the experimental and theoretical curves.

1. Introduction

Self-organized quantum dot structures formed in Ill-V materials have attracted an increasing interest due to many possible applications in optoelectronics. It offers a possibility to fabricate, for example, InAs quantum dots on GaAs substrate can be in a successive growth process, including the formation of coherent structure of InAs islands and the overgrowth of GaAs cap layer by molecular beam epitaxy (MBE). The height and size of the InAs quantum dots are functions of InAs layer thickness and the deposition conditions. It is reported that the quantum dot superlattices can be formed by alternating growth of the GaAs and strained InAs layers by the alignment of the coherent strained islands [1].

Up to now, many authors have investigated self-organized quantum dot structures by experimental methods [2-5]. The X-ray diffraction measurements were also used to investigate this system [6]. In this work, a multilayer structure model was established in order to get more satisfactory fitting of the experimental results. Based on the simulation of the dynamic theory, the height of InAs quantum dots and the average strain in the GaAs cap layer were determined.

2. Experiments and Discussion

A series of samples with different InAs coverages were grown by a V80H MKII MBE system. As InAs thickness exceeded the 1.7 ML, a change of reflected high energy electron diffraction (RHEED) pattern from streak to spot indicated the formation of a coherent InAs island. Transmission electron microscope (TEM) observations have also confirmed this result [7]. The structure parameters of the sample were designed as in Table 1. X-ray experiments were carried out by using Rigaku SLX-LA double crystal X-ray diffractometer on a conventional 12 kW X-ray generator. Monocrystal Ge with asymmetrical (004) reflection was used as monochromator and the copper target was chosen ($\lambda_{K\alpha1}$=1.5405 Å).

Fig. 1 shows three (004) diffraction curves with increasing thicknesses of InAs layers, 1 ML (a), 3 ML (b), and 6 ML (c), respectively. The interference fringes are caused by the phase shift between the cap GaAs layer and the GaAs substrate. The effective phase shift depends on the thickness of the strained layer [8]. In curve (a), the pendellosung fringes appear symmetrically around the substrate peak and the oscillation of the fringes is the most strong among the three curves. As the InAs layer thickness increases (curves (b) and (c)), the intensity and the visibility of the fringes on the right side of the substrate peak become weaker making the whole pattern asymmetric. The fringes become less obvious, especially for curve (c), in which the oscillations can be well distinguished only in a magnified scale as shown in the inset of Fig. 1. According to the fringe distances,

Table 1 Structure parameters

Thickness	Sample #1	Sample #2	Sample #3
InAs(ML) layer	1.0	3.0	6.0
GAAs cap layer (nm)	designed: 90.0 measured: 89.7	designed: 90.0 measured: 88.3	designed: 90.0 measured: 80.0

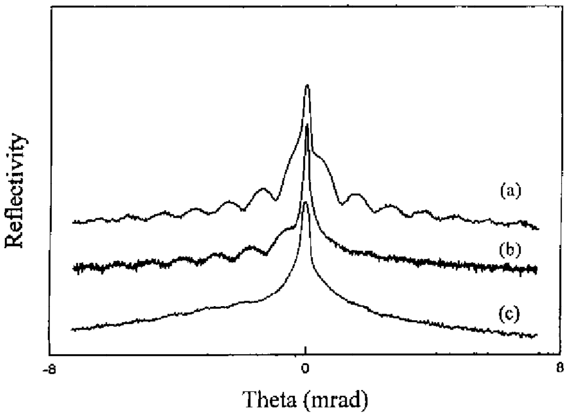

Fig. 1 (004) X-ray diffraction patterns with different thicknesses of InAs interlayers. The designed thicknesses of InAs are (a) d_{InAs}=1.0 ML; (b) d_{InAs}=3.0 ML; (c) d_{InAs}=6.0 ML.

the GaAs cap layer thicknesses are determined for three samples and are shown in Table 1.

Experimental and simulating (004) diffraction patterns of 1 ML InAs are shown in Fig. 2 (a) and (b), respectively. X-ray dynamic diffraction theory [9] and a 2D InAs strained layer model are employed for theory [9] and a 2D InAs strained layer model are employed for simulation. Since the theoretical curve fits quite well with the experimental curve, it is reasonable to consider that the InAs interlayer of this sample is in the case of 2D growth (proved also by RHEED and TEM) [7]. It is also indicates that X-ray dynamic diffraction theory can be successfully employed to investigate the InAs 2D layered-growth as some previous work [10]. The thicknesses of InAs and GaAs cap layers are 1.1 ML, 897.OA, respectively. In the meantime, it is noted that the experimental curves of (b) and (c) (shown in Fig. 1) are not symmetric and the interference fringes move to the lower angle. According to the RHEED and TEM results [7], the three dimensional (3D) InAs island occurred in sample #2 and #3. Furthermore, the same simulation process as curve (a) (shown in Fig. 2) is employed, in which the InAs layer is considered as 2D layered-growth, but no satisfactory agreement can be obtained. In reference [6], a misfit of peak position between the experimental and theoretical curves can be observed. Therefore, the asymmetry is attributed to the formation of InAs island. A strain distribution, which is different from the case of 2D layered-growth, should be considered in order to get a better simulation.

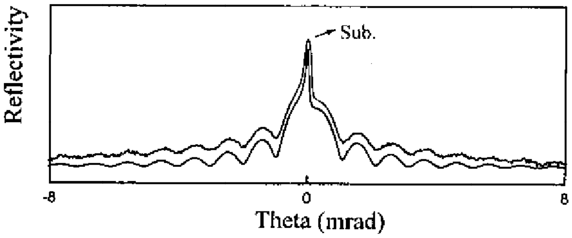

Fig. 2 Experimental (a) and theoretical (b) curves of sample #1. The calculated thicknesses are d_{InAs} = 1.1ML and $d_{GaAs(cap)}$ = 89.7 nm respectively.

For the sample #2 which is correspondent to the curve (b) in Fig. 1, we make simulation by using X-ray dynamic theory and a “multilayer structure model', as shown in Fig. 3. Since a large lattice mismatch exists between InAs and GaAs layers, and the islanding allows some elastic relaxation of the strain [11] (shown in Fig. 3), the strained InAs islands will form spontaneously. These islands are three dimensionally epitaxial and coherently strained (i.e. no dislocations). During the successful growth, the GaAs would deposit at the valley region between the InAs islands firstly (part B in Fig. 3). In the vicinity of InAs island, the GaAs would be compressed in the lateral direction and elongated in the vertical direction (part A in Fig. 3) to match the InAs unit cell. In meanwhile, the lattice would be strongly deformed around InAs islands. In part B, the GaAs unit cell would be expended in the lateral direction to keep the total number of unit cells in this direction. Therefore, the unit cells of GaAs are changing from compressed near the InAs island to expanded at the center region of two InAs islands (i.e. from part A to B in Fig. 3). Otherwise, misfit dislocations will produce. After the valley regions are full filled, the GaAs will deposit on the both regions, the top of InAs islands and GaAs valleys. The GaAs unit cells on the top of InAs island (part C in Fig. 3) will tend to a coherent growth with the [InAs island and hence have small expansion in the lateral direction due to the elastic relaxation with the InAs unit cell. This may also cause the GaAs being compressive along the lateral direction in part D (see Fig. 3). When the X-ray projects on the regions including part A and C (see Fig. 3), the phase shift depends on the island shape and will not keep constant as shown in Fig. 4, in which the island shape comes from atomic force microscope (AFM) results [121. The optical path 1 and 2 are not the same when X-ray passes through the InAs island. Therefore, it is reasonable to conclude that the Pendellosung fringes do not appear by this reason. On the contrary, the lattice will be less deformed in the region including part B and D due to a relatively far away from the InAs island (see Fig. 3). As the X-ray penetrates this region, the phase shift can nearly keep constant and can be considered as the source for the pendellosung fringes. The region included the GaAs cap layer, the tensile GaAs layer (part B in Fig. 3), the compressive GaAs layer (part D in Fig. 3), 1 ML InAs wetting layer and the substrate, can be considered as a “multilayer structure" model. Based on this “multilayer structure" model, simulation is carried out. A perfect agreement is obtained between the experimental and theoretical curves, as shown in Fig. 5. The main feature of the Xray diffraction pattern (i.e. the shape and the shift of pendellosung fringes) is well reproduced in the calculated curve. The simulated parameters, the thicknesses and the average strain of part B and D are dB=5.0 nm, dD= 2.1 nm, eB'=-0.03, ED'=O.013, respectively.

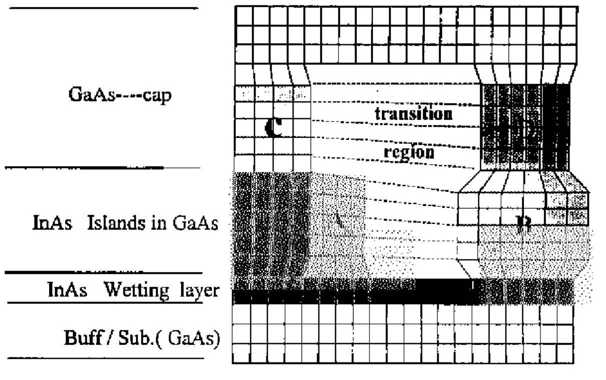

Fig. 3 A schematic drawing of the growth process of a quantum dot (beneath Part C). Part A and D are the compressed GaAs regions. Part B and C are the tensile GaAs regions.

According to the TEM observations, when the InAs layer thickness increases from 3 to 6 ML, the size of the InAs islands does not expand, but the density corresponding with island arises. The increase of density implies that the flat region of the GaAs layer between the InAs islands (part B and D in Fig. 3) will reduce, which leads up to the intensity decrease of the interfere strings as shown in Fig. 1. Furthermore, the regions B and D become more distorted to cause the interfere fringes oscillation weaker.

The thickness of compressive GaAs layer (part B in Fig. 3) can be estimated as the average height of

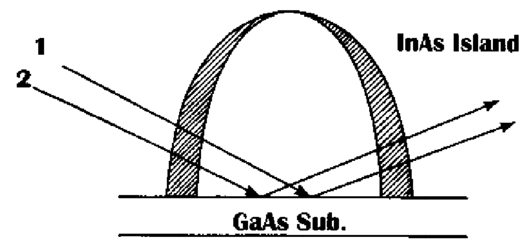

Fig. 4 Diagram of optical path as X-ray projects on the InAs island. The shadow represents the strong deformation region around InAs island. The optical paths for X-ray 1 and 2 are different and depended on the shape of InAs island.

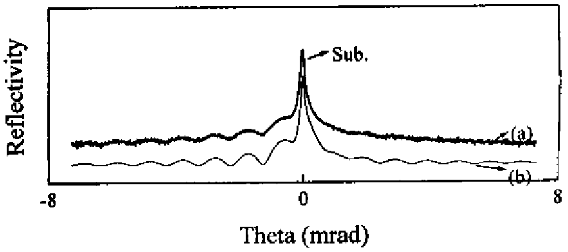

Fig. 5 Experimental (a) and theoretical (b) curves of sample #2. The calculated thicknesses and average strains of the two parts corresponding to Fig. 4 are d_B=5.0 nm, d_D=2.1 nm, $\varepsilon_B^{\perp}$=-0.03, $\varepsilon_D^{\perp}$=0.013, $d_{GaAs(cap)}$=88.3 nm.

InAs islands. Actually, no homogeneous strain (compressive or tensile) or/and well defined layer thickness exist in the sample since the strain in the epitaxial GaAs layer varies gradually. However, we can obtain an average strain and a height of InAs island in sample #2. Our results show qualitatively that compressive and tensile GaAs regions should exist between InAs islands.

3. Conclusion

In summary, HRDCD is a powerful tool to investigate the buried InAs quantum dot structures. A multilayer structure model is employed to successfully explain asymmetry of the Pendellosung fringes, the shift of peak position and the amplitude reduction. The height of InAs quantum dots can be estimated by the simulation based on X-ray dynamic theory. As InAs 3D growth happens, both a tensile and a compressive GaAs regions may occur between InAs islands.

Reference

[1] J. Tersoff, C. Teichert and M. G. Legally, *Phys. Rev. Lett.*, Vol. **76**, No. 10 (1996), 1675-1678.

[2] H. Kitabayashi, T. Waho, *J. Cryst. Growth*, **150** (1995), 152-157.

[3] P. Chen, Q. Xie, A. Madhudar, Li Chen and A. Konkar, *J. Vac. Sci. Technol.*, **B12**(4) (1994), 2568-2573.

[4] A. Tackeuchi, Y. Nakata, S. Muto, Y. Sugiyama, T. lnata and N. Yokoyama, *Jpn. J. Appl. Phys.* Vol. **34** (1995), L405-407.

[5] J. Y. Marzin, J. M. Gerard, A. Izrael and D. Barrier, *Phys. Rev. Lett.*, Vol. **73**, No. 5 (1994), 716-719.

[6] A. Krost, F. Heinrichsdorff, D. Bimberg, A. [Darhuber and G. Bauer, *Appl. Phys. Lett.* **68**(6) (1996), 785-787.

[7] X. R Yang, W. Zhang, Z. G. Chen, J. F. Tian and H. Z. Zheng, *Chinese J. Semiconductors* Vol. **17**, No. 11 (1996) 869-873.

[8] L. Tapfer, M. Ospelt and H. von Kanel, *J. Appl. Phys.*, **67**,1298 (1990).

[9] Y. Zhuang, Y. T. Wang, D. S. Jiang, X. R Yang, X. M. Jiang, J. Y. Wu, L. S. Xiu and W. L. Zheng, *Appl. Phys. Lett*., **68**(8) (1996),1147-1149.

[10] A. Mazuelas, L. Gonzalez, L. Tapfer and F. Briones, *Mat. Res. Soc. Symp. Proc.*, Vol. **263** (1992), 473-477.

[11] D. J. Eagelsham and M. Cerullo, *Phys. Rev. Lett.*, **64**, 1943 (1990).

[12] Q. H. Xie, R Chen, A. Kalburg, T. R. Ramachandran, A. Nayfonov, A. Konkar and A. Madhukar, *J. Cryst. Growth*, **150** (1995), 357-363.