The Rigaku Journal
Vol. 14/ number 1/ 1997

# STUDY OF THE STRUCTURES OF AN ASYMMETRICALLY COUPLED DOUBLE-WELL SUPERLATTICE BY DOUBLE-CRYSTAL X-RAY DIFFRACTION

W.Q. MA, Y. ZHUANG, Y.T. WANG, AND D.S. JIANG

National Research Center for Optoelectronic Technology, and Institute of Semiconductors, Chinese Academy of Sciences, P.O. Box 912, Beijing 100083, China

An asymmetrically coupled (GaAs/AlAs/GaAs/AlAs)/GaAs(00l) double-well superlattice is studied by HRDCD. It is found that the intensity of satellite peaks is modulated by wave packet of different sublayers. In the course of simulation, the satellite peaks in the vicinity of the node points of wave packet are very informative for precise determination of sublayer thickness and for improving simulation accuracy.

The structural characteristics of superlattice are probably the most important and fundamental parameters because the physical and device properties strongly depend on them.

Therefore great enthusiasm and efforts have been devoted to precise characterization of superiattices. High resolution double-crystal X-ray diffraction (HRDCD) plays an indispensable role in determining the structure of superlattice precisely due to its high resolution, nondestructiveness, and almost no sample preparation [1]. At present, the HRDCD method is widely accepted. The usual process is to obtain the structural parameters by fitting the experimental results according to X-ray dynamic or kinematic theories. Although many papers have been reported about the superlattice including 2 sublayers in one period, investigations to superlattice including 4 sublayer in one period are still rare because in the case of superlattice with 4 sublayers in one period, the contribution of different sublayer to diffraction pattern intermingles and results in a complicated so-called “satellite-peak modulation phenomenon” and thus it is much more difficult to analyse and simulate.

In this paper, we invesitigate an asymmetric GaAs/AlAs/GaAs/AlAs double-well superlattice. The experimental curve is simulated by X-ray dynamic theoryn [2, 3] which is regarded more precise and trustworthy than kinematic theory [4, 5] due to its consideration of interactions between the incident and the reflected wave. But its physical image is not so clear and direct. Therefore a “wave packet method” based on kinematic theory, which is considered to have clearly physical image, is employed to explain the complicated satellite-peak modulation phenomenon. It is also found that the satellite peaks in the vicinity of “node points of wave packet” are especially beneficial to precise determination of sublayer thickness and enhancing the accuracy of simulation.

The sample is a 20-period asymmetric GaAs/AlAs/GaAs/AlAs double-well superiattice which is grown on a semi-insulating GaAs substrate of (001) orientation by molecular beam epitaxy (MBE). The respective thicknesses of wells and barriers are deliberately designed asymmetric. It has been reported that such a structure forms type-I-type-II mixed double quantum wells in which free-carrier scattering is the dominant scattering mechanism and the carrier concentration can be adjusted within a relatively wide range [6]. So the precise determination of different sublayer is very crucial.

HRDCD experiment is carried out by Rigaku SLX-LA diffractometer whose 12 kW X-ray generator is RU-20OBH. The copper target is used and X-ray wavelength is 1.54051 Å. Figure 1 is the schematic diagram of the experimental setup for the measurement. The Ge (004) asymmetric diffraction monochromator is employed as the first crystal. The measurement is completed by $\theta/2\theta$ scan mode and the resolution of rotation angle $\theta$ is 0.001°. The employed voltage and current are 50 kV and 150 mA, respectively. In order to promote the accuracy of measurement, step-scan mode is used.

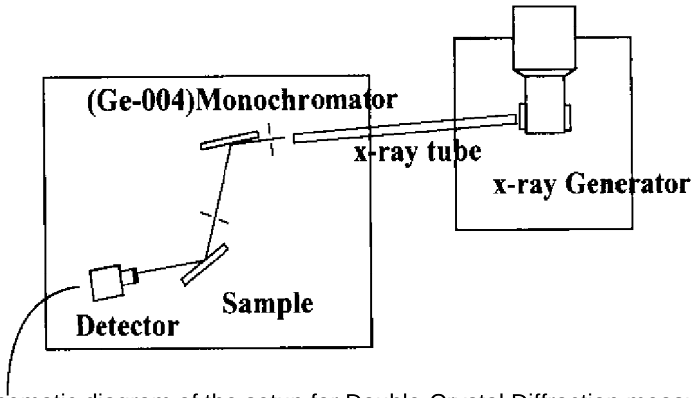


**Fig.1**. Schematic diagram of the setup for Double-Crystal Diffraction measurement.

According to the dynamic theory, the total reflective amplitude of (00h) diffraction for a N-layer heterostructure $R_{h,N,T}$ is:

$$R_{h,N,T}= [ R_{h,N}+ R_{h,N-1,T}(T_{h,N}T_{h,N}- R^{h,N}R_{h,N})]/(1 - R_{h,N-1,T}R_{h,N}) \quad (1)$$

where $R_{h,N}$ and $T_{h,N}$ are reflective and transmissive amplitude of the N-th layer for (00h) diffraction, respectively. Here

$$R_h = \xi_1\xi_2\left(C_1 - C_2\right) / \left(C_2\xi_2 - C_1\xi_1\right) \quad (2)$$

$$T_h = C_1C_2\left(\xi_1 - \xi_2\right) / \left(C_2\xi_2 - C_1\xi_1\right) \quad (3)$$

$$\xi_{1,2} = \left(-z \pm \sqrt{\left(q + z^2\right)}\right) / \chi_h \quad (4)$$

$$Y_j = -\sqrt{\frac{\gamma_0}{|\gamma_h|}}\,\frac{\pi V_j \sin^2\theta_B \Delta\omega}{r_e\lambda^2|F_j|} \quad (5)$$

$$C_{1,2} = \exp\left(-i\phi_{1,2}t\right) \quad (6)$$

$$q = b\chi_h\chi_h \quad (7)$$

$$b = \gamma_0 / \gamma_h \quad (8)$$

$$z = \sin\left(2\theta_B\right)\cdot\Delta\omega \quad (9)$$

$$\begin{aligned}\Delta\omega = \theta - \theta_B + \left(\varepsilon^{\perp}\cos^2\alpha + \varepsilon^{||}\sin^2\alpha\right)\tan\theta_B \\ \pm\left(\varepsilon^{\perp} - \varepsilon^{||}\right)\sin\alpha\cos\alpha\end{aligned} \quad (10)$$

where $\chi_0$ and $\chi_h$ are the 0-th and h-th Fourier coefficients of polarizability, respectively, $\lambda$ is the X-ray wavelength ($\lambda$=1.54051 Å); b is asymmetry factor, $\gamma_0$ and $\gamma_h$ are direction cosines of the incident and diffracted waves, respectively; $\theta_B$ is the kinematic Bragg angle, t is the thickness of N-th layer; $\alpha$ is the angle between crystal surface and reflection plane; $\varepsilon^{\perp}$ and $\varepsilon^{||}$ are the strains perpendicular and parallel to the crystal surface, respectively.

The period of superlattice is obtained according to experimental curve by equation below:

$$D = \frac{\lambda|\gamma_h|}{\Delta\theta\sin\left(2\theta_B\right)} \quad (11)$$

where $\Delta\theta$ is the angular spacing between two satellite peaks.

Keeping the period of superlattice constant, we fit the experimental results using X-ray dynamic theory. Although the thickness value of each sublayer can be obtained by simulation, the resolution and accuracy are still unsatisfactory. So the “wave packet method” based on X-ray diffraction kinematic theory, which is regarded to have a more clearly physical image, is used to solve the problems mentioned above.

The reflective amplitude of an N-period superlattice with four sublayers A, B, C, D in one period according to X-ray diffraction kinematic theory is:

$$I = \gamma_0 / |\gamma_h| \frac{\sin^2\left[N\left(\Phi_A + \Phi_B + \Phi_C + \Phi_D\right)\right]}{\sin^2\left[\left(\Phi_A + \Phi_B + \Phi_C + \Phi_D\right)\right]} I' \quad (12)$$

where

$$I' = I_1 + I_2 + I_3 \quad (13)$$

$$I_1 = \Psi_A^2 + \Psi_B^2 + \Psi_C^2 + \Psi_D^2 \quad (14)$$

$$I_2 = 2\Psi_A\Psi_B\cos(\Phi_A+\Phi_B) + 2\Psi_B\Psi_C\cos(\Phi_B+\Phi_C) + 2\Psi_C\Psi_D\cos(\Phi_C+\Phi_D) \quad (15)$$

$$I_3 = 2\Psi_A\Psi_C\cos(\Phi_A+2\Phi_B+\Phi_\chi) + 2\Psi_B\Psi_D\cos(\Phi_B+2\Phi_C+\Phi_d) + 2\Psi_A\Psi_D\cos(\Phi_A+2\Phi_B+2\Phi_C+\Phi_D) \quad (16)$$

$$\Phi_j = A_j Y_j \quad (17)$$

$$A_j = \frac{r_e\lambda|F_j|t_j}{V_j\sqrt{\gamma_0|\gamma_h|}} \quad (18)$$

$$Y_j = -\sqrt{\frac{\gamma_0}{|\gamma_h|}}\,\frac{\pi V_j\sin 2\theta_B\Delta\omega_j}{r_e\lambda^2|F_j|} \quad (19)$$

$$\Delta\omega_j = \theta-\theta_B + \left(\varepsilon_j^{\perp}\cos^2\alpha + \varepsilon_j^{||}\sin^2\alpha\right)\tan\theta_B \pm \left(\varepsilon_j^{\perp}-\varepsilon_j^{||}\right)\sin\alpha\cos\alpha \quad (20)$$

$$\Psi_j = \frac{\sin\Phi_j}{Y_j} \quad (21)$$

Here r, is the classical electron radius; $F_j$, $V_j$, and $t_j$ are the j-th layer structure factor, volume of the unit cell, and thickness, respectively. $\varepsilon^{\perp}_j$ and $\varepsilon^{||}_j$ are the j-th layer strains perpendicular and parallel to the surface. Other parameters coincide with that of the preceding in its represented meaning. In equation (21), $\Psi_j = \sin\Phi_j / Y_j$, is the wave packet of the j-th layer which is analogous to the diffraction amplitude of a single epitaxy layer. From equation (12), when $\sum\Phi_j / Y_j = n\pi$, the diffraction intensity appears to be maximum and the corresponding angles are the positions of satellite peaks of superlattice, but it also can be seen that the diffraction intensity is modulated by different wave packet in one period which forms intensity modulation phenomenon of satellite peaks.

When $\Phi_j = n\pi$, i.e., $\Psi_j = 0$, the corresponding angles are called the "node points of the modulation wave for j-th sublayer". It is found that, in the vicinity of the node point, $\Psi_j$ varies very sensitively with $\Delta\omega$, i.e., when $\Phi_j \to n\pi$ the variation of the intensity I' primarily comes from the variation of $\Psi_j$ and other sublayer's modulation wave packets only contribute to I' slightly. Thus, if we choose the satellite peaks in the vicinity of the node points of j-th sublayer wave packet to simulate, the other sublayer's effects on I' can be nearly removed and a accurate thickness of j-th sublayer can be obtained. Similarly, the accurate parameters of other sublayers can also be obtained.

In Fig. 2, a and b represent experimental curves and the final simulated curve by dynamic theory. The final result for GaAs/AlAs/ GaAs/AlAs layer thickness in one period is:

| GaAs | AlAs | GaAs | AlAs |
|---|---|---|---|
| 27 Å | 107 Å | 78 Å | 210 Å |

In can be seen that the ± 4th satellite peaks and ±8th satellite peaks are almost extinct. In Fig. 3, a, b, c, d represent wave packet of GaAs (27 Å), AlAs (107 Å), GaAs (78 Å), AlAs (210 Å), respectively; e is wave packet when one period is regarded as one layer, i.e.,

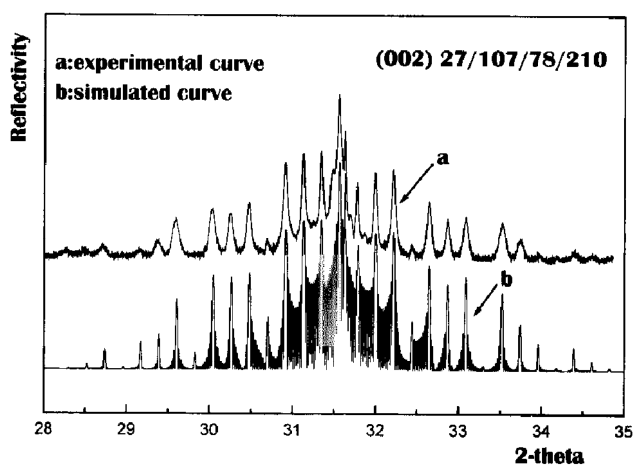


**Fig. 2**. Experimental (a) and simulated curve (b) of (002) diffraction.

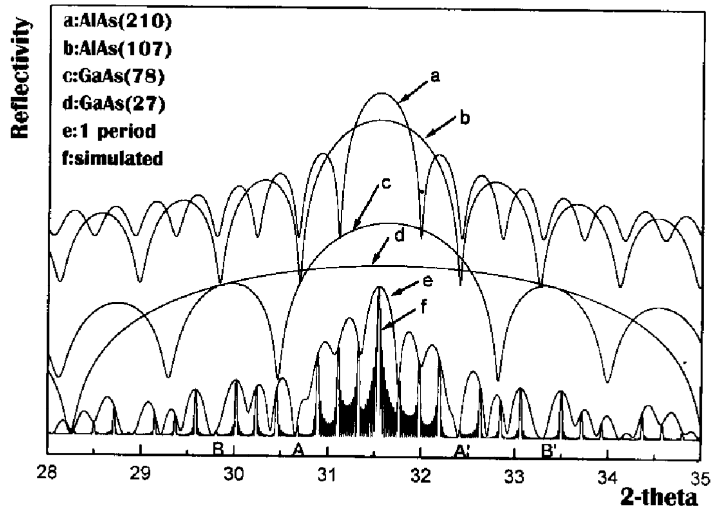


**Fig. 3**. Wave packet of different sublayer. a: AlAs (210 Å), b: AlAs (107 Å), c: GaAs (78 Å), d: GaAs (27 Å), e: 1 period, f: simulated curve of kinematic theory.

the wave packet of one superlattiice period and f is the simulated curve by kinematic theory. The points A, A' and B, B' in Fig. 3 are node point of AlAs (210 Å), AlAs (1 07 Å) wave packet, corresponding to the ±4th and ± 8th satellite peaks, respectively. If we adjust AlAs (210 Å) sublayer thickness with a deviation from 210 Å of only 1Å, the resulted variation of simulated curve will be quite pronounced. Comparing simulated curve with experimental curve, it is found that there is a best agreement between two curves when the thickness of AlAs is 210 Å. Therefore it indicates that the thickness of the AlAs sublayer is 210 Å with 1 Å resolution. In the same way, the thickness of other sublayer can also be decided. It is obvious that the agreement between simulated and experimental curves is nearly perfect, thus it is believed that the method we employed is worthy of reliable.

In summary, that a simulation of X-ray diffraction pattern of complicated SL structures based on dynamic theory and combining with wave packet method gives satisfactory results.

# References


[1] L. Tapfer et al., *J. Appl. Phys*., **67**, 1298 (1990).

[2] W. J. Bartels, J. Hornstra and D. J. W. Lobeek, *Acta Cryst*., **A 42**, 539 (1986)

[3] L. Tapfer and K. Ploog, *Phys. Rev*., **B 40**, 9802 (1989).

[4] V. V. Speriosu, *J. Appl. Phys*., **52**, 6094 (1981).

[5] V. S. Speriosu and T Vreeland, Jr., *J. Appl. Phys*., **56**, 1591 (1984).

[6] Wei Liu, Desheng Jiang et al., *Appl. Phys. Lett*., **67**, 679 (1995).