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Structural Investigation of InGaAs/InP Quantum Wire Array Using Triple-Axis X-ray Diffractometry

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Abstract InGaAs/InP quantum wire array are investigated by X-ray triple-axis diffractometry and the reciprocal space contour mapping for (00h) diffraction. X-ray dynamic theory is employed to simulate the reciprocal space contour mapping of quantum wires. The structural parameters and strain states are determined. A good agreement between the experimental and simulated mapping is obtained.

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High resolution X-ray diffractometry is a very important and indispensable tool for characterization of epitaxial layers, hetero-structural and superlattices due to its non-destructiveness and high resolution. It is well known that X-ray diffraction is a very effective means in obtaining the information of the structures grown perpendicular to the sample surface. Quite recently, it has been found that X-ray diffraction is also suitable for the investigation of periodical laterally-corrugated structures such as semiconductor quantum wires and quantum dots because it can provide the information about geometric parameters, strain states and the information of the side wall roughness and destruction of quan-

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tum wires, especially when the two-dimensional reciprocal space contour mapping (RSCM) by triple-axis system is obtained[1].

Triple-axis X-ray diffraction is a new-developed method, appearing and developing only in recent years. It is known that the standard double-axis X-ray diffractometry uses an open detector and therefore integrates the scattering from the specimen over all angles within its aperture[2]. So it swamps the information of orientation distribution and that of lattice spacing distribution[3]. It is difficult to unravel different contributions to intensity, such as those of rough surface and from perfect crystal scattering. The detector probe in double-axis diffraction is a line with a certain width and the detector probe in triple-axis diffraction can be in principle regarded as a line of zero width, i.e., a δ function probe[4]. Triple-axis diffraction can distinguish contributions to intensity from mosaic spread (ω scan mode) and from lattice spacing distribution (ω-2θ scan mode). The RSCM is obtained by performing a series of independent of ω-2θ scans, in which ω (angle between the incident X-rays and the sample surface) and 2θ (angle between the wave vectors of the incident and diffracted X-rays) vary independently.

In our investigations on the InGaAs/InP quantum wires, we measured RSCM of an array of quantum wires. The sample is started from the growth of an InGaAs layer on InP substrate by metalorganic chemical vapor phase deposition (MOCVD). Then it is patterned by photolithography on the sample surface by the interference of two coherent He-Cd laser beams. In the course of photolithography, dry etching is employed. The exposure light of a He-Cd laser is devided by a beam-splitter into two beams. They are reflected by the reflective mirrors and then reach on the surface of the specimen and interfere to cause an exposure of photo-resist. The wavelength of He-Cd laser employed is 352nm. Afterwards, an array of quantum wires is formed by the etching processing.

The X-ray experiments are carried out by Rigaku SLX-1A diffractometer whose 12kW X-ray generator is RU-200BH. A copper target is used and X-ray wavelength is 0.15405nm. The Ge (004) asymmetric diffraction monochromator is employed as the first crystal. The Si (220) diffraction is used as analyzer which is mounted in the front of the detector. In order to obtain RSCM, the independent variation of two scanning angles ω and 2θ should be fulfilled. The resolution of ω is 0.005° and that of 2θ is 0.008°. The employed voltage and current are 50kV and 150mA, respectively.

In this paper, X-ray dynamic theory[5,6] is used to simulate the RSCM of quantum wires. It is usually thought that X-ray dynamic theory is only applicable to the case of an infinite plane, therefore it seems that it would not be applicable to the laterally corrugated structures such as quantum wires. But if one layer of periodical corrugated multi-layer structure is regarded as an one-dimensional array of crystal cells and its structure factor is calculated as a whole, the dynamic theory should be applicable. Based on this idea, a rectangle model is employed for quantum wires. Supposing that the period and the width of wires are p and d, respectively, the structure factor of one crystal cell for (hkl) diffraction

$F_{hkl,s}$ is shown below:

$$F_{hkl,s} = \sum_j f_j e^{2\pi i(hx_j + ky_j + lz_j)} \tag{1}$$

where f_j is the scattering factor of the j-th atom in one crystal cell and (x_j, y_j, z_j) denotes its position. For $(00h)$ diffraction, the structure factor of wires for one period $F_{00h,p}$ is calculated below:

$$F_{00h,p} = F_{00h,s}(1 + e^{2\pi ih\,a} + e^{2\pi ih\,2a} + \cdots + e^{2\pi ih[\frac{d}{a}]}) \tag{2}$$

where a is the lattice constant and $[\frac{d}{a}]$ denotes the integer part of quotient of $\frac{d}{a}$. The structure factor of whole single layer F_w is shown below:

$$F_w = F_{00h,p} \sum_{j=0}^{\infty} {}^{2\pi ih\,jp} = \frac{F_{00h,p}}{1 - e^{2\pi ihp}} \tag{3}$$

F_w is the structure factor used in dynamic theory. The thickness of respective layer for multi-layer has been automatically included in the calculation of dynamic theory. X-ray dynamic theory is suitable for the treatment of multi-layer structure. Therefore, the above model can deal with quantum wires of multi-layer structure.

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

$$R_{h,N,T} = [R_{h,N} + R_{h,N-1,T}(T_{h,N}T_{h,N} - R_{h,N}R_{h,N})]/(1 - R_{h,N-1,T}R_{h,N}) \tag{4}$$

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

In the course of measurements, the direction of wires should be adjusted to be perpendicular to X-ray diffraction plane. If the direction of wires is parallel to the diffraction plane, the satellite peaks of wires will not appear. This can be understood if X-ray diffraction of wires is regarded as a multi-slit Fraunhofer diffraction[6]. Fig. 1 is the result of experimental RSCM of the sample for (004) diffraction. W0, W ±1 and W ±2 denote 0-th, ±1st, and

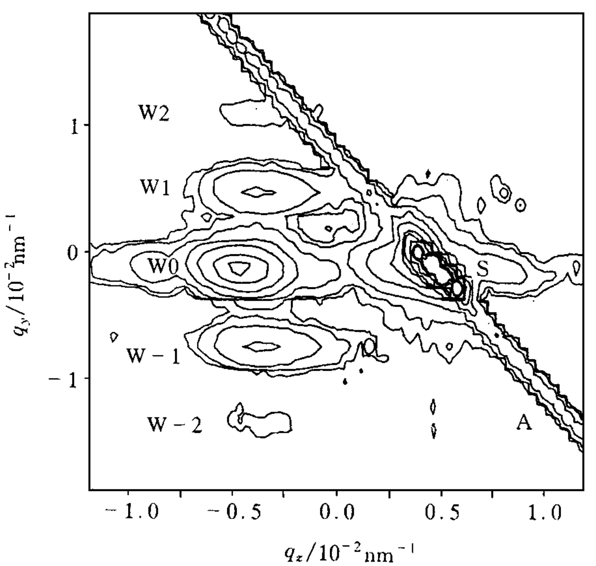

Fig. 1 2-dimensional reciprocal space contour mapping (RSCM) of the quantum wire array

±2nd satellite peaks of wires, respectively. "S" is the peak of substrate and "A" is an artifact, the so-called "analyzer streak" and will be neglected in the further discussions. It can be seen that ±2nd satellite peaks of wires exist although they are very weak. The RSCM can provide more information than the pattern of double-axis diffraction. According to the spacing of satellite peaks of wires along the q_y direction, the period of wires can be obtained[7].

$$p = |n_1 - n_2|\lambda\cos(\theta_e)/[\Delta\theta_{n_1,n_2}\sin(2\theta_B)] \quad (5)$$

where n_1 and n_2 denote the n_1-th and n_2-th satellite peaks. θ_e is the angle between diffracted beam and the surface of sample. θ_B is the Bragg angle and $\Delta\theta_{n_1,n_2}$ is the spacing between n_1-th and n_2-th satellite peaks. From Fig. 1 it can be decided that the period of wires is 240 nm and the depth of wires does not reach the surface of substrate, otherwise there should appear satellite peaks of wires along the q_y direction around substrate peak additionally.

In Fig. 1 there is a distinct shift of the 0-th satellite peak to the InP substrate peak along the negative q_z direction comparing with as-grown sample. It shows that the perpendicular strain in wires has been changed after wires are fabricated on the substrate surface. We have also measured a pattern of double-axis diffraction. Fig. 2 (see last page) is the (004) diffraction pattern of as-grown InGaAs epilayer on InP substrate for comparison. It is confirmed that the epilayer is of high quality judged by the appearance of interference fringes. The spacing between the peak of epilayer and substrate peak in Fig. 2 is 387 arc second instead of 610 arc second in Fig. 1. It indicates that the strain along growth direction wires becomes larger than that of as-grown sample, namely, the average lattice constant becomes greater. It can be understood because the stresses along both the growth direction and the direction perpendicular to wires after fabrication of wires are zero, i.e., there are two free directions while in the as-grown epilayer only the growth direction is free. The formation of wires has changed the conditions of the surface system.

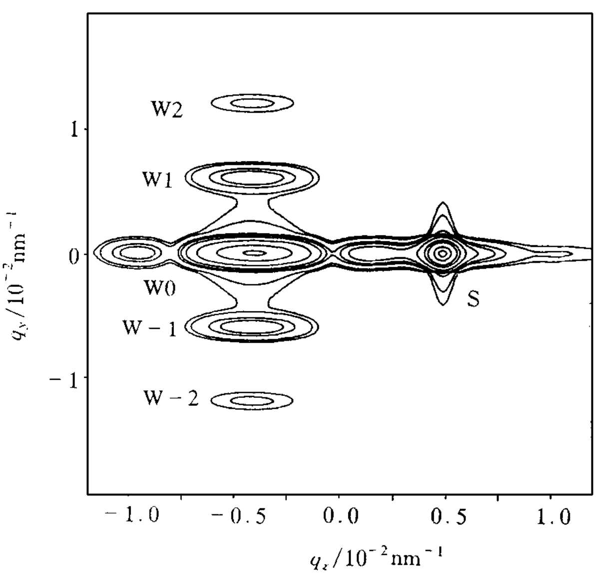

Fig. 3 Simulated RSCM result according to the dynamic theory

Fig. 3 is the simulated RSCM according to the dynamic theory. The simulated depth and width of wires are 100nm and 110nm, respectively.

The parameters used in the simulation are in accordance with the observations of scanning electronic microscope (SEM) (Fig. 4, see last page). It is found that there is a good agreement between the experimental and simulated mapping.

In summary, triple-axis diffraction is a very useful and important method and reciprocal space contour mapping can supply useful information for the analysis of the structural properties of quantum wires much more than double-axis diffraction pattern, especially for quantum wires. X-ray dynamic theory is used to simulate the RSCM and a good agreement between experiment and simulation is obtained.

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