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G-7-2

Cross-Sectional Evolution and Its Mechanism during Selective MBE Growth of GaAs Quantum Wires on (111)B Substrates

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1. Introduction

High density arrays and networks of quantum dots (QDs) and quantum wires (QWRs) are required for realization of next generation high density quantum LSIs. Selective MBE growth on pre-patterned substrates is one of the most promising techniques for formation of such structures in size- and position-controlled fashion.

Recently, in view of application to hexagonal binary decision diagram (BDD) quantum LSIs [1], our group has demonstrated feasibility of growth of hexagonal AlGaAs/ GaAs QWR networks on (111)B GaAs substrates by selective MBE[2]. Three fold symmetry of the (111) plane is inherently favorable for formation of hexagonal QWR networks with smooth wire connection, and is advantageous for high-density integration of BDD node devices having three branches. However, selective growth process on a non-planar (111)B substrate is complicated due to kinetics involving high-index facets. Thus, proper understanding of the growth mode and mechanism is indispensable for precise control of growth.

The purpose of this paper is to investigate, both experimentally and theoretically, evolution of wire cross-section and its mechanism during selective growth of <-1-12>-oriented QWRs on (111)B patterned substrates.

2. Experimental

The substrate pattern used in this study is shown in **Fig. 1(a).** It consists of <-1-12>-orientated straight mesa stripes that were prepared by electron-beam (EB) lithography and HBr-based wet chemical etching. Hexagons can be formed by using <-1-12> and other two equivalent orientations.

Wet chemical surface treatments in the atmosphere and thermal cleaning under an As pressure in the MBE chamber were applied prior to growth. Typical material supply for MBE growth is shown in **Fig. 1(b)**. First, GaAs buffer layer was grown on patterned substrates in order to prepare initial growth template for selective growth. Then, molecular beams for planar growth of an $Al_{0.3}Ga_{0.7}As$/GaAs/ $Al_{0.3}Ga_{0.7}As$ sandwiched layer were supplied on the buffer template, and this led to formation of embedded GaAs QWRs. The V/III ratio was 10, and the growth temperatures, T_{sub}, was from 640°C to 700°C. The growth rate of AlGaAs was 1000nm/hour for planar growth.

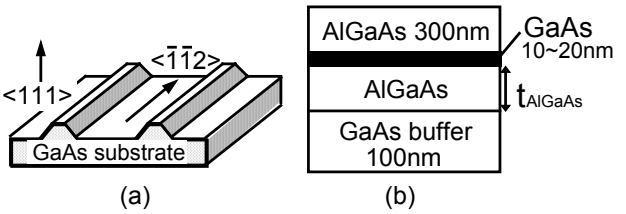

Fig. 1 (a) Patterned substrate and (b) material supply used in this study.

3. Results and Discussion

1) Cross-sectional structure of wire

A cross-sectional SEM image of a grown QWR is shown in **Fig.2(a)** together with its schematic illustration in **Fig2(b)**. Growth of GaAs buffer led to formation of flat-top mesa structures defined by the top (111)B facet and side (5-12) facets. After the entire growth, embedded GaAs nanowires were selectively formed on the top (111)B facet with a reduced lateral size, as seen in **Fig. 2(a)**.

2) Change of wire width and position with time

In order to see the change of wire width and position with growth time, a repeated wire growth experiment was carried out with a constant interval. The result is shown in **Fig.3(a)**. It is seen that the lateral wire width, W, of the wire and position changes linearly with time, remarkably keeping previous growth history. The observed change of the wire width with time is summarized in **Fig.3(b)**.

A closer look revealed that the wire is determined by two boundaries between the region grown on the top (111)B facet and the regions grown on the side (5-12) facets. As shown by a dotted line in **Fig.3(a)**, these

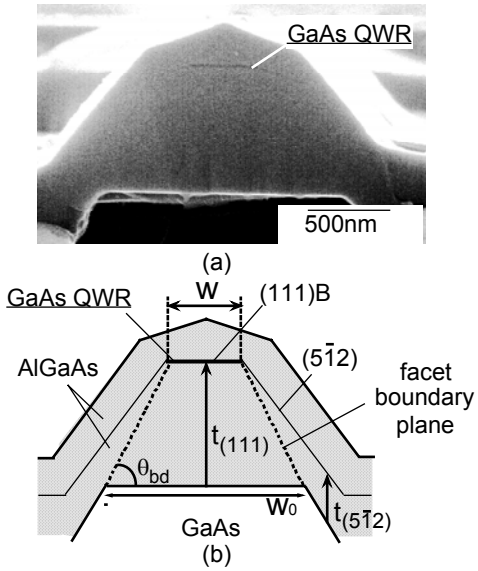

Fig. 2 (a) Cross sectional SEM image of <-1-12>-oriented GaAs QWR and (b) its schematic.

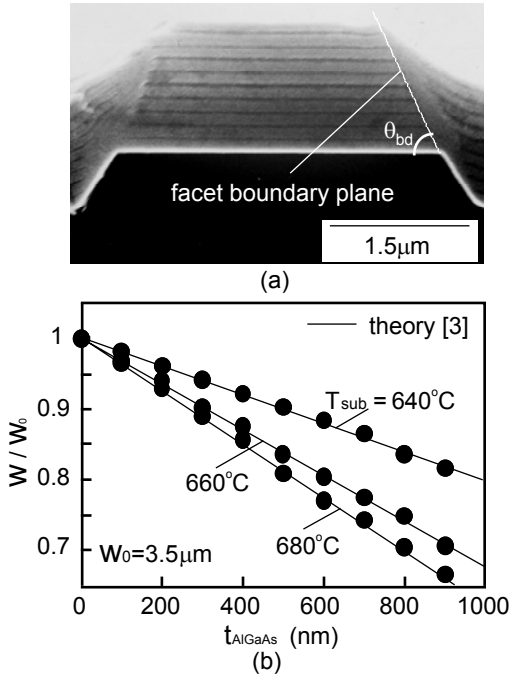

Fig. 3 (a) Wire cross-section after repeated growth of QWRs and (b) normalized wire width vs. AlGaAs supply thickness.

boundaries maintain a constant angle, θ_{bd}, with respect to the (111)B plane during entire growth, and form what we called "facet boundary planes (FBPs)" in our previous work on wire growth on (001) patterned substrates [3]. Since growth underneath both facets proceeds linearly with time following FBPs, the wire width and wire position change linearly with time or the thickness of the AlGaAs barrier layer grown underneath, as seen in **Fig. 3(b)** for width.

FBPs did not correspond to any of high index crystalline facets, but were determined by growth kinetics. Thus, its angle, θ_{bd}, with respect to the substrate plane changed with the growth temperature, T_{sub}.

In order to further achieve quantitative data for evolutions of wire cross-setion, the vertical growth rates on different facets were measured, changing the growth temperature. The measured growth rates, $t_{(111)}$and $t_{(5\text{-}12)}$, defined in **Fig. 2(b)** and their ratios are plotted in **Fig.4** as a function of the growth temperature, T_{sub}. Here, the values of $t_{(111)}$and $t_{(5\text{-}12)}$ are normalized by the growth rate on the planar (111)B substrate. The growth rate on the side (5-12) facets decreased strongly with increase of T_{sub}. This led to increase of $t_{(111)}/t_{(5\text{-}12)}$ ratio at higher temperatures, resulting in the increase of the growth selectivity. This explains the faster reduction of wire width at higher temperatures seen in **Fig. 3(b).** Using the data in **Fig.4**, the cross-sectional features of grown QWRs can be quantitatively predicted using the formulas we derived for growth on (001) substrates[3].

3)Computer simulation of the growth process

In order further to understand and quantify the growth kinetics, a computer simulation was attempted using the following phenomenological equation.

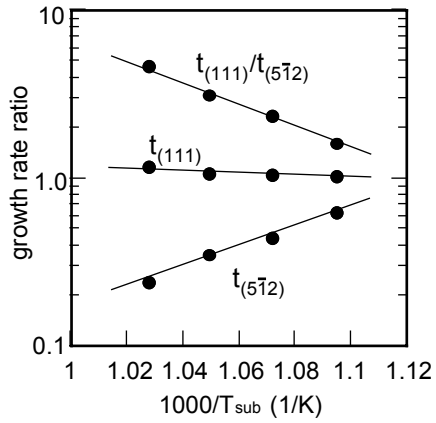

Fig. 4 Growth rates and their ratio vs. growth temperature T_{sub}.

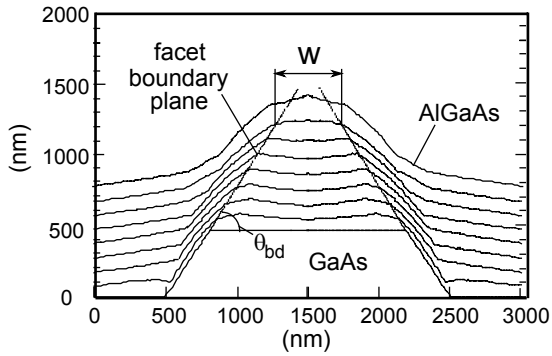

Fig.5 Simulated growth profile for <-1-12>-oriented QWR.

$$\frac{\mathrm{d}n}{\mathrm{d}t} = G \cdot \cos\theta - \frac{n}{\tau} - \frac{\mathrm{d}J}{\mathrm{d}x} \qquad (1),$$

$$J = -D\frac{n}{kT_{sub}} \cdot \mathrm{grad}(U) \qquad (2)$$

where n is the adatom density, G is the molecular beam flux and J is the surface diffusion flux of adatoms. τ, D and U are life time until incorporation, surface diffusion coefficient and chemical potential of adatoms on a facet, respectively. These parameters were taken to be functions of growth temperature, T_{sub}, and facet angle, θ.

An example of calculated growth profile is shown in **Fig.5.** The facet boundary planes are clearly reproduced by simulation. Theoretically obtained value of θ_{bd} showed good agreements with the experiment.

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