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Surface reconstructions and reflection high-energy electron diffraction intensity oscillations during homoepitaxial growth on nonmisoriented GaAs(111)B by MBE*

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Abstract: The growth by molecular beam epitaxy of high quality GaAs epilayers on nonmisoriented GaAs(111)B substrates is reported. Growth control of the GaAs epilayers is achieved via *in situ*, real time measurement of the specular beam intensity of reflection high-energy electron diffraction (RHEED). Static surface phase maps of GaAs(111)B have been generated for a variety of incident As flux and substrate temperature conditions. The dependence of GaAs(111)B surface reconstruction phases on growth parameters is discussed. The ($\sqrt{19}\times\sqrt{19}$) surface reconstruction is identified to be the optimum starting surface for the latter growth of mirror-smooth epilayers. Regimes of growth conditions are optimized in terms of the static surface phase diagram and the temporal RHEED intensity oscillations.

Key words: GaAs(111)B; RHEED; surface reconstruction; epilayer
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1. Introduction

Recently, the study of epitaxial growth on GaAs(111)B substrates has received much attention due to special properties of the (111) orientation, such as a large piezoelectric effect and high light emitting efficiency[1]. These properties suggest the possibility of fabricating novel optoelectronic devices with strong piezoelectrically generated internal fields and low threshold current lasers[2, 3]. For the actual device applications, it is crucial to provide high quality epitaxial films on GaAs(111)B substrates. In the literature, few reports have been focused on epitaxial growth on GaAs (111) surfaces compared to the (100) orientation. Furthermore, films grown on GaAs(111)B often show rough surface morphologies, presented as threefold pyramids, and other types of defects[4, 5]. Among several methods employed to deposit these films, molecular beam epitaxy (MBE) has been found to be rather difficult. Moreover, it has been found that the homoepitaxial growth is highly sensitive to growth parameters and the grown surfaces are easily marred by pyramid-like structures[6]. To the best of our knowledge, little work has been done on the growth of GaAs epilayers with a specular surface on nonmisoriented (111)B substrates, especially via the conventional MBE.

In the present work, we report the growth control achieved via *in situ*, real time monitoring of the specular beam intensity of RHEED on static and dynamic GaAs(111)B surfaces. GaAs films with specular surfaces are successfully obtained on nonmisoriented GaAs(111)B substrates by conventional MBE. A phase diagram was introduced to describe the dependence of GaAs(111)B surface reconstruction phases on growth parameters. The dependence of surface morphology and crystal quality on growth conditions was discussed in terms of RHEED dynamic behavior as well as growth parameters.

2. Experimental procedure

The epitaxial growth experiments were performed in a Riber 32P MBE system. The sample temperatures were obtained by calibrating the substrate heater thermocouple with an Ircon V Series optical pyrometer. The arsenic and gallium flux

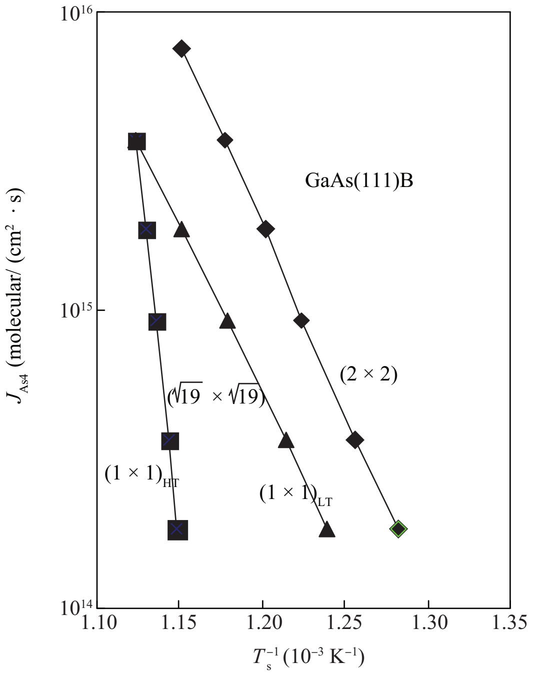

Fig. 1. GaAs (111)B surface static phase diagram.

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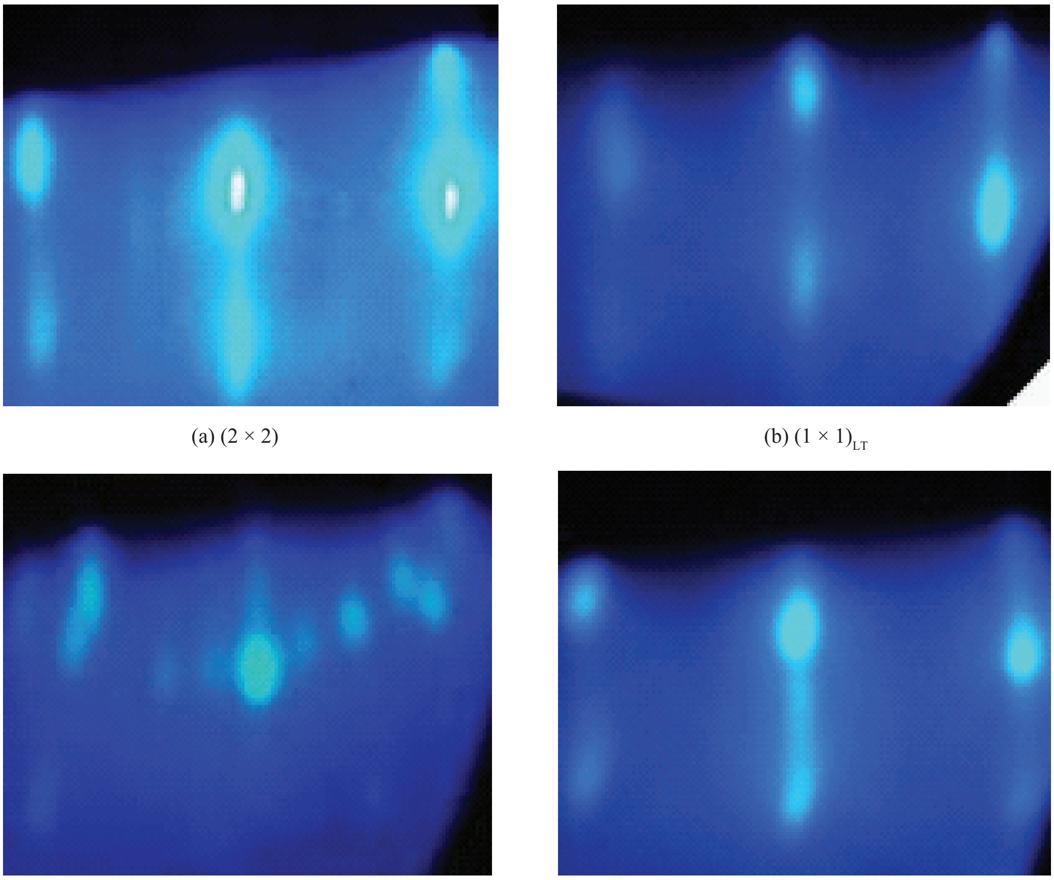

(a) (2×2) (b) $(1\times1)_{LT}$

(c) $(\sqrt{19}\times\sqrt{19})$ (d) $(1\times1)_{HT}$

Fig. 2. RHEED pattern of the GaAs(111)B surface.

measurements were performed with an ion gauge. The various surface reconstructions during the growth process were monitored *in situ* using a Riber 100 15KV RHEED system.

Undoped nonmisoriented GaAs(111)B substrates were employed herein for the study. The substrates were prepared using standard degreasing steps and then cleaned in hot sulfuric acid and cold sulfuric acid, and etched in a 5:1:1 solution of sulfuric acid, hydrogen peroxide and deionized water. After etching, the wafers were rinsed with deionized water and blown dry with N_2 gas. GaAs(111)B substrates together with a (100) wafer were bonded with indium solder on molybdenum platters and then introduced into the reactor. As a complementary method of substrate temperature calibration, the static GaAs(100) (2×4) to c(4×4) reversible transition surface phase, carried out under the conditions with $T_{sub} = 525 \pm 5$ ℃, As_4 flux $J_{As_4} \approx 5\times10^{14}$ molecular/(cm^2·s), was observed by RHEED.

3. Results and discussion

3.1. Surface phase diagram

The four surface phases existing in the GaAs(111)B material system are $(1\times1)_{HT}$, $(\sqrt{19}\times\sqrt{19})$, $(1\times1)_{LT}$ and (2×2) reconstructions. The two phases labeled $(1\times1)_{HT}$ and $(1\times1)_{IT}$ represent a high temperature and a low temperature (1×1) phase, respectively. During the epitaxial growth on GaAs (111) surfaces, according to the research of Yang *et al.*[7], when the chemisorbed surface coverage of As $\theta > 0.72$, the RHEED pattern corresponding to 2×2 reconstruction is observed. For the lower As surface coverage ($\theta < 0.58$), the $\sqrt{19}\times\sqrt{19}$ reconstruction RHEED pattern appears. As increasing the substrate temperature and reducing the V/III ratio, there exists $\theta_{(2\times2)} > \theta_{(1\times1)LT} > \theta_{(\sqrt{19}\times\sqrt{19})} > \theta_{(1\times1)HT}$, i.e., the surface reconstruction on GaAs(111)B transforms from an As-rich to a Ga-rich phase.

Under the static (i.e., $J_{Ga} = 0$) conditions, five As_4 flux conditions ranging from 10^{14} to 10^{16} molecular/(cm^2·s) were employed for the experiments. The substrate temperatures were selected randomly within the range of 400 ℃ $< T_s <$ 700 ℃. The static surface maps of GaAs(111)B generated from the RHEED data in this current study are shown in Fig. 1. It is clear from the figure that the phase maps are divided into four regions corresponding to GaAs(111)B $(1\times1)_{HT}$, $(\sqrt{19}\times\sqrt{19})$, $(1\times1)_{LT}$ and (2×2) surface reconstruction, respectively. It can also be seen that there exists a critical incident As_4 flux of $J^c_{As4} = 5\times10^{15}$ molecular/(cm^2·s). As the As_4 flux exceeds J^c_{As4}, the $\sqrt{19}\times\sqrt{19}$ reconstruction phase is quenched, and, in the meantime, the $(1\times1)_{HT}$ and the $(1\times1)_{LT}$ reconstructions are linked together to form a single (1×1) surface phase.

4. Effect of various starting surfaces on epitaxial growth

Figure 2 shows a series of RHEED photographs, taken at various substrate temperatures under a constant As_4 flux

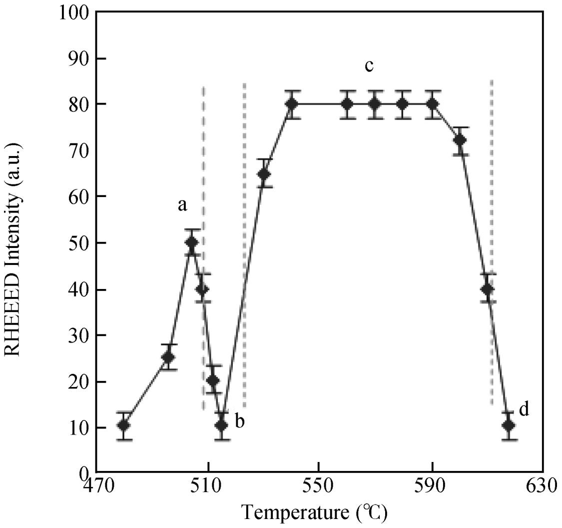

Fig. 3. RHEED intensity diagram of a GaAs(111)B static surface phase.

$J_{As_4} = 2 \times 10^{15}$ molecular/(cm^2·s), of the four static GaAs(111)B surface phases: (2×2), $(1 \times 1)_{LT}$, $(\sqrt{19} \times \sqrt{19})$ and $(1 \times 1)_{HT}$. The corresponding RHEED specular beam intensity dependence on the substrate temperature is shown in Fig. 3. The electron beam is along the $\langle 110 \rangle$ direction. The dashed lines indicate the phase-transition lines of the four surface reconstructions. Based on the dynamical diffraction theory, the higher intensity of the diffraction streaks we observe, the lower surface step density and surface roughness are obtained[8, 9]. From Fig. 3, it can be seen that the diffraction in the plateau region of GaAs(111)B-$(\sqrt{19} \times \sqrt{19})$ exhibits the highest RHEED intensity. This attests that the $\sqrt{19} \times \sqrt{19}$ starting surface regime is propitious to growing mirror-smooth epilayers.

5. Behaviour of RHEED oscillations under different growth parameters

A number of GaAs films were grown under arsenic pressure $J_{As_4} = 1 \times 10^{15}$ molecular/(cm^2·s), R_g = 0.2 ML/s and with different substrate temperatures. The growth parameter dependence of the intensity oscillations is revealed by the real-time RHEED measurements. Figure 4 shows the RHEED intensity oscillations on GaAs(111)B along the $\langle 110 \rangle$ direction at different growth temperatures. Curves *a*–*g* correspond to the film growth at substrate temperatures of 520–580 ℃, respectively. It is shown that the RHEED patterns for the films grown at 520, 530 and 540 ℃ exhibit lower diffraction intensity, which indicates rough surface morphologies. This can be ascribed to the decrease in evaporation rate of chemisorbed As from the surface and the cation migration length at low growth temperatures. By comparing the resulting films, the size and density of the surface pyramids decrease with increasing substrate temperature. However, as the temperature increases further, as seen in Fig. 4(*g*), the degradation in surface morphology occurs, which is due to the decrease in As surface coverage and the disappearance of $\sqrt{19} \times \sqrt{19}$ surface reconstruction. Hence, the proper substrate temperature for the epitaxial growth is in the range of 550–580 ℃.

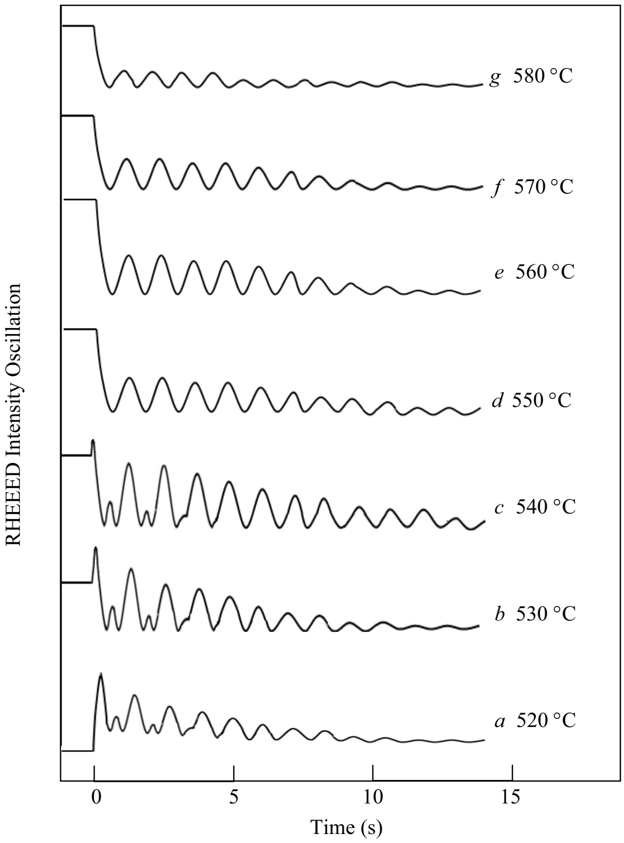

Fig. 4. RHEED intensity oscillations on GaAs(111)B at different T_s.

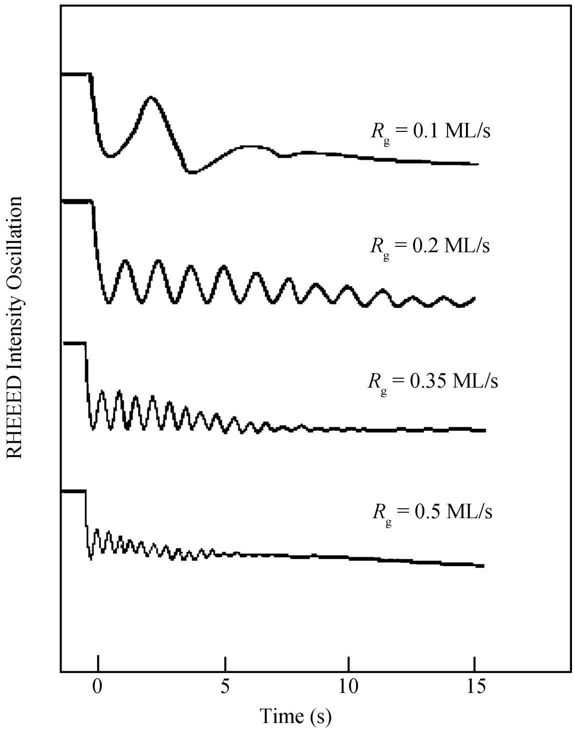

Fig. 5. RHEED intensity oscillations on GaAs(111)B with different R_g.

Figure 5 shows the RHEED intensity oscillations under different growth rates R_g. It is clear from the figure that the in-

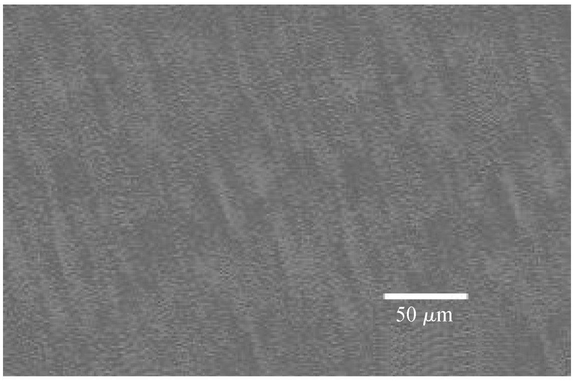

Fig. 6. Nomarski micrograph of the surface morphology of a GaAs(111)B epitaxial layer.

tensity oscillation for the growth under R_g = 0.1 ML/s is not obvious and it is hard to distinguish the oscillation period from the pattern. With increasing growth rate, for R_g = 0.2, 0.35 and 0.5 ML/s, the oscillations disappear after several periods and the intensities reach a steady state. It can also be seen that the steady-state intensities of the samples with R_g = 0.2, 0.35 and 0.5 ML/s decrease with elevating R_g. According to the morphology observations of the resulting films, it is found that the density and size of pyramids increase with increasing growth rate. This increase results from the Ga surface migration length decreasing under high Ga flux, which induces the destruction of two-dimensional growth mode. So it is essential to grow epilayers with a specular surface at a relatively low growth rate.

In addition, each As atom in the top layer of GaAs(111)B could easily form three bonds to the underlying Ga atoms. Hence, under higher As_4 flux, Ga atoms may have more chances of bonding As and depositing on the surface. Correspondingly, the surface migration length of the Ga atoms decreases, which results in an increase in the surface step-density. Based on the above analysis, lower As_4 flux may improve the surface morphologies of the resulting films.

5.1. Growth of epilayers with a mirrorlike surface

GaAs epilayers, approximately 1000 Å thick, grown with a $\sqrt{19} \times \sqrt{19}$ starting surface at a substrate temperature of 570 ℃ with growth rate R_g = 0.25 ML/s and arsenic pressure $J_{\mathrm{As}_4} = 1 \times 10^{15}$ molecular/(cm^2·s), were successfully obtained on GaAs(111)B substrates. The surface morphology was observed under a Nomarski microscope. As shown in Fig. 6, there are no pyramids and the film appears mirror smooth to the naked eye.

6. Conclusions

GaAs epilayers with a specular surface are successfully achieved on nonmisoriented GaAs(111)B substrates via conventional MBE. A surface reconstruction phase diagram has been introduced to give a more complete description of GaAs(111)B growth under static conditions. The optimal growth conditions are discussed in terms of the static surface phase diagram and the temporal specular beam intensity.

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