Orderly Array of In-Plane GaAs Nanowires on Exact (001) Silicon for Antiphase-Domain-Free GaAs Thin Films

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Abstract

We report material characterization of antiphase-domain-free GaAs thin films grown out of highly ordered in-plane GaAs nanowires on exact (001) silicon substrates. The evolution of surface morphology from the nanowires to the thin films has been investigated by SEM. Anisotropic defect distribution and the impact of the initial nanowire quality on the resultant coalesced layers have been analyzed by TEM, XRD and AFM. The growth scheme in this work opens up a promising path to integrate GaAs based devices on the CMOS-compatible Si platform.

INTRODUCTION

In the past few years, there has been a growing interest in heteroepitaxy of III-V nanostructured materials on lattice-mismatched Si substrates, aiming to integrate mainstream Si technologies with III-V functionalities. A great emphasis of recent research has been directed toward selective area growth on pre-patterned Si using the aspect ratio trapping process [1-2], in which the defects originated from the large lattice mismatch can presumably be blocked by the dielectric sidewalls. Recent studies also suggest that the use of a V-grooved Si (111) surface is beneficial to restrict the generation of antiphase-domains and further enhance the defect trapping efficiency [3-4]. So far, high crystalline quality III-V channel materials for nanoscale transistors have been integrated on Si using this approach. However, the very small volume of useful materials in the growth cavities between dielectrics limits this technique in photonic device applications which typically require a larger active area [5]. In this respect, we recently demonstrated an innovative growth scheme for achieving antiphase-domain-free GaAs thin films on exact (001) silicon using highly ordered in-plane GaAs nanowires formed by the aspect ratio trapping method [6]. Thanks to the combined advantages from nanopatterned growth and epitaxial lateral overgrowth, low defect density, large-area GaAs thin films can be obtained on industrial-standard Si substrates. In this paper, we carried out detailed characterization regarding the evolution of morphology and defect density from the nanowires to the coalesced GaAs layers using SEM, AFM and XRD. The defect trapping effect has been studied by TEM. The influence of the initial nanowire quality on the resultant thin films was also analyzed.

MATERIAL GROWTH

N-type on-axis Si (001) substrates were used in the experiments. A 160 nm thick SiO$_2$ layer was first formed on the Si substrates. [110] direction oriented stripe pattern with an opening width of 90 nm and a line pitch of 130 nm was realized by top-down lithography and dry etching process. After surface cleaning using RCA-1 solution and native oxide removal by diluted HF, the sample was immediately immersed in a 70 °C heated KOH solution (45%) to etch the Si surface. [111] facets were revealed at the bottom of the trenches as a result of the lowest Si etch rates in {111} planes.

The material growth was carried out using a low-pressure (100 mbar) metal-organic chemical vapor deposition system with a horizontal reactor. TEGa and TBA were used as group-III and group-V sources. After a thermal cleaning step at 800 °C in the reactor, selective area growth of GaAs nanowires was carried out using a two-step growth procedure that consists of a low-temperature nucleation layer and a high-temperature main layer. Fig. 1 illustrates the gas flow and temperature sequence for the planar nanowire growth on Si. Fig. 2 shows a 70° tilted-view SEM image of an orderly array of GaAs nanowires with a height of 150 nm. High position-controllability, good uniformity and smooth {111} top facets have been demonstrated.

![Fig.1 Schematic illustration of gas flow and temperature sequence for the planar GaAs nanowire growth on Si. (note: LT = low temperature, HT = high temperature)](image-url)

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Prior to the coalesced thin film growth, the SiO₂ walls defining the stripes were removed by buffered oxide etch. Epitaxial lateral overgrowth was conducted at 600 °C using TEGa and AsH₃ as sources. SEM was used to monitor the surface morphology evolution. Fig. 3(a) displays the initial closely-pitched nanowires without SiO₂ in between. When observed after overgrowth of a 60 nm GaAs layer, these high density nanowires merged together, forming a bumpy surface morphology, as shown by Fig. 3(b). Fig. 3(c) and (d) are cross-sectional SEM images of the coalesced GaAs films on the V-grooved Si after overgrowth of 300 nm and 900 nm-thick layers, indicating a flat surface has been reached.

**DEFECT ANALYSIS**

The crystalline quality of the planar GaAs wires and thin films was examined by TEM and XRD. The TEM specimens were prepared using conventional mechanical thinning, followed by ion beam milling. A JEOL2010F field-emission microscope operating at 200 keV was used for the TEM observation. Fig. 4(a) displays a cross-sectional TEM image of the array of GaAs nanowires with a height of 200 nm taken along the [110] zone axis. We found only a few {111} plane stacking faults in the bulk of the GaAs nanowires. The TEM images in Fig. 4(b) and (c) with higher magnification highlighted the hetero-interface between GaAs and Si. The large lattice mismatch was accommodated by the formation of a few nanometer-thick stacking-disordered layers instead of threading dislocations that propagate. Fig. 4(d) presents cross-sectional TEM image of the coalesced GaAs thin film with a thickness of about 900 nm. Most of the defects at the GaAs/Si interfacial region have been trapped by the V-grooved concaves.

XRD θ-rocking curves were measured by an Empyrean HRXRD system working at 40 kV voltage and 40 mA current. A hybrid monochromator consisted of an x-ray mirror and a two-crystal Ge (220) two-bounce monochromator provides an intense and line-collimated x-ray beam with Cu Kα1 radiation. A channel-cut Ge analyzer crystal is placed in front of the detector to reduce angular acceptance. We found asymmetric FWHMs of the rocking curves depending on the direction of the incident line-focused x-ray beam with respect to the sample azimuth. Fig. 5 presents the measured FWHMs from the nanowires to the coalesced thin films with the x-ray beam aligned perpendicular and parallel to the stripes. The initial nanowires with a height of 150 nm exhibited an FWHM of 450 and 615 arcsec in the perpendicular and the parallel
directions, respectively. At the early stage of lateral overgrowth, a slight increase of rocking curve FWHM was observed, which suggested the emergence of coalescence defects. With further increased overgrowth thickness, the FWHM in the perpendicular direction decreased rapidly and surpassed the FWHM in the parallel direction. The 900 nm GaAs on V-grooved Si achieved an FWHM as small as 238 arcsec, indicating good crystalline quality. Fig. 6 displays AFM image of 900 nm coalesced GaAs film with a scanned area of 5×5 μm². We found spiral patterns and a few straight lines related to stacking faults, but no antiphase-domain boundaries. A root-mean-square roughness of 3.1 nm was achieved from the AFM measurement.

The quality of the nanowires at the beginning can have significant impact on the resulting coalesced thin films. Fig. 7(a) shows a tilted-view SEM image of a GaAs nanowire array with “notch-like” structural defects. These features are believed to be related to stacking faults caused by the rough edges of the V-grooves. Higher density defects manifest themselves in the broadening of θ−rocking curves. Compared to the nanowires shown in Fig. 2, The FWHM is 50% and 10% larger in the perpendicular and parallel directions respectively. After coalescence growth of GaAs thin film on these relatively more defective nanowires, we found more stacking faults appearing as [110] direction orientated dashed line in the AFM image, shown by Fig. 7(b).

CONCLUSIONS

In conclusion, we reported growth of low defect density GaAs thin films on V-grooved (001) silicon using orderly arrays of in-plane nanowires as a “special” buffer. The morphology and defect evolution from the nanowires to the thin films have been investigated in detail by SEM, XRD, TEM and AFM. The small linewidths of the XRD rocking curve FWHM from the GaAs nanowires to thin films with x-ray aligned perpendicular and parallel to the stripes.
curves and the antiphase-domain-free surface morphology suggest the great potential of using nanowire array to fabricate high quality GaAs-on-Si compliant substrates for monolithic integration of III-V devices on Si.

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REFERENCES

ACRONYMS
SEM: Scanning Electron Microscopy
TEM: Transmission Electron Microscopy
XRD: X-ray Diffraction
AFM: Atomic Force Microscopy
CMOS: Complementary Metal Oxide Semiconductor
TEGa: Triethylgallium
TBA: Tertiarybutylarsine
FWHM: Full-width-at-half-maximum