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Elimination of APBs in a GaAs layer directly-grown on an on-axis Si(001) substrate by optimizing an AlGaAs nucleation layer

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Abstract

The direct growth of III-V compound semiconductor on Si(001) is an unsolved problem for monolithically integrated photonic devices on the Si platform. Here, we report the high quality growth of GaAs layer on on-axis Si(001) substrates. Single domain GaAs layer was grown on top of a AlGaAs nucleation layer on Si(001) substrate. By optimizing Al content of the nucleation layer, anti-phase domains (APDs) were self-eliminated at GaAs layer. This result represents a key step towards the realization of monolithically integration of III-V devices on silicon platform.

1. Introduction

Epitaxial growth of III-V compound semiconductor on Si substrates has attracted attention as a monolithic integration method for high performance optical devices[1–3]. Recently, this method is also thought as a core technology for integrating light sources of silicon photonics technology to overcome the limitation of metal wiring in an integrated circuit[4,5]. However, due to differences in crystal properties (lattice constant, polarity-nonpolarity, thermal expansion coefficient) between III-V semiconductors and Si, they cause crystal defects such as anti-phase boundaries (APDs), dislocations and cracks. APB is a boundary formed by Ga-Ga bond and As-As bond when GaAs, which is a polar material, is grown on Si, which is a nonpolar material. Since the injected carriers extinct at the local charge of the APB, the electrical characteristics of the sample containing the APB deteriorates. In addition, high-density defects are formed because the strain is concentrated in APBs. In order to remove the formed APB, the same regions of the crystal axes need to be adjacent to each other. Since the formed APBs are difficult to remove, a method of suppressing the formation of APB by using an off-axis Si substrate has been used[6–8]. However, off-axis Si substrates do not have CMOS compatibility, then, they are not suitable for fabrication of Si photonics devices.

In this paper, we report a successful elimination method of APBs in GaAs layer on an on-axis Si(001) substrate by optimizing an AlGaAs nucleation layer.

2. Experimental method

All the samples were grown by conventional solid-source molecular beam epitaxy (MBE) system (VG semicon V80H). Arsenic tetramer (As_4) was supplied from valved cracking cell. High resistance n-type on-axis Si (001) substrates were used for this study. A native oxide layer (~2 nm) on the Si wafer was removed with diluted hydrogen fluoride acid (DHF). After loading to the growth chamber, the Si wafer was normally pre-heated at 950°C for 10 min.

40 nm-thick $Al_xGa_{(1-x)}As$ with each Al composition x (x=0 (sample A), 0.3 (sample B), 0.5 (sample C), 0.7 (sample D)) were grown on Si. 800 mm-thick GaAs was grown on each sample to evaluate the APB annihilated thickness, the RMS roughness of the GaAs surface, and the FWHM of the XRD ω-2θ. For evaluating dislocation density of samples, quantum dot (QD) layer sandwiched by two AlGaAs clad layer was additionally grown on 2.3 μm-thick GaAs layer. Figure 1 shows schematic illustration of the PL structure grown on an on-axis Si(001) substrate. After etching with NH_4OH based etchant, Cross-sectional SEM was used for observing elimination of APBs. We performed macro-photoluminescence (PL) spectroscopy on the grown QDs at room temperatures. Conventional semi-conductor laser light at 632 nm was employed for pumping the samples.

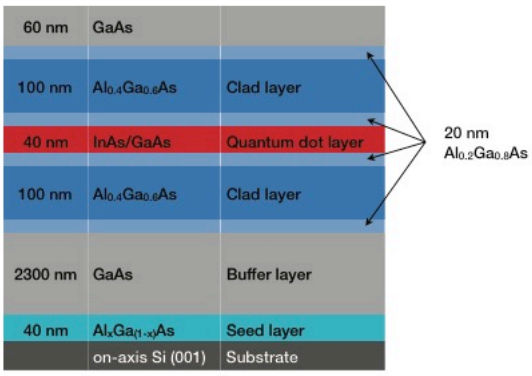

Fig. 1 Schematic illustration of the structure grown on a Si(001) substrate.

3. Results and Discussion

Figure 2 shows cross-sectional SEM images of sample B and sample D. For sample B (x = 0.3), the APB disappears in the region near the nucleation layer. However, in sample D (x = 0.7), the APB is extended to the GaAs surface. This phenomenon becomes clear on the surface observation of a sample grown with 800 nm GaAs. Figure 3 shows AFM images of samples A and D. In the surface image of Sample D, there is GaAs surface with high roughness and many APDs different from the image of the surface of sample A. Figure 4 shows dependence of Al composition of nucleation layer with APD annihilated thickness, RMS roughness and XRD ω-2θ full-width-half-maximum (FWHM). The PL emission intensity from the QD structure on Sample B is two times brighter than that on Sample A. From a comprehensive point of view, GaAs buffer layer in sample B has the highest crystal quality. This method is considered to form a low-density grain boundary, because large nucleation grains grow in a short time under the longer migration length condition of adatom.

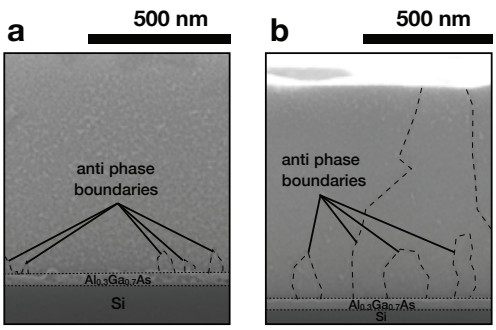

Fig. 2 Cross-sectional SEM images of GaAs layer on (a) $Al_{0.3}Ga_{0.7}As$ nucleation layer and (b) $Al_{0.7}Ga_{0.3}As$ nucleation layer grown on Si(001) substrate.

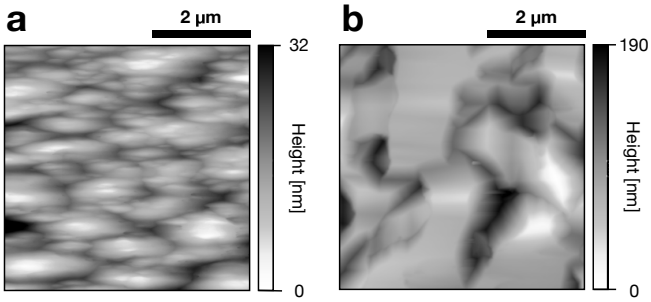

Fig. 3 AFM images of GaAs layer on (a) $Al_{0.3}Ga_{0.7}As$ nucleation layer and (b) $Al_{0.7}Ga_{0.3}As$ nucleation layer grown on Si(001) substrate.

4. Conclusion

We have successfully demonstrated the direct growth of GaAs on on-axis Si (001) substrates. By optimizing Al content of nucleation layer to 30%, the high crystal quality of grown GaAs was obtained on the nucleation layer. This monolithic approach will open the way toward facile integration of III-V devices into Si-based platform.

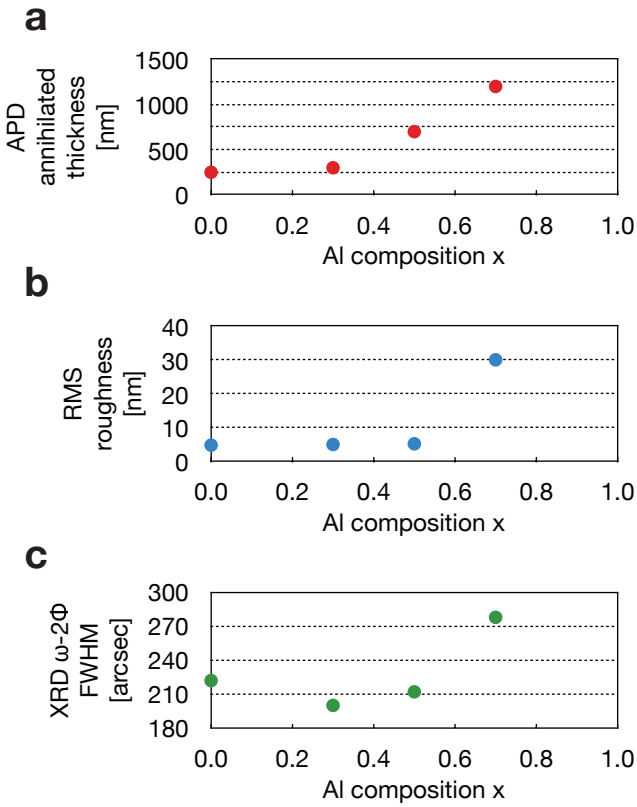

Fig. 4 Dependence of Al composition (x) of nucleation layer and (a) APD annihilated thickness, (b) RMS roughness and (c) XRD ω-2θ FWHM.

Acknowledgements

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