Effects of AlAs interfacial layer on material and optical properties of GaAs/Ge(100) epitaxy

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(Received 4 February 2008; accepted 20 March 2008; published online 8 April 2008)

GaAs/AlAs/Ge(100) samples grown at 650 °C with AlAs interfacial layer thickness of 0, 10, 20, and 30 nm were characterized using transmission electron microscopy, secondary ion mass spectrometry (SIMS), and photoluminescence (PL) techniques. SIMS results indicate that the presence of an ultrathin AlAs interfacial layer at the GaAs/Ge interface has dramatically blocked the cross diffusion of Ge, Ga, and As atoms, attributed to the higher Al–As bonding energy. The optical quality of the GaAs epitaxy with a thin AlAs interfacial layer is found to be improved with complete elimination of PL originated from Ge-based complexes, in corroboration with SIMS results. © 2008 American Institute of Physics. [DOI: 10.1063/1.2908042]

Recently, there has been renewed interest in monolithic integration of GaAs with Ge for the use in metal-oxide-semiconductor field-effect-transistors (MOSFETs) due to the higher electron mobilities in GaAs as compared to the elemental semiconductors such as Si and Ge. It has been thought that the ideal next-generation complementary MOSFETs would consist of GaAs n-MOSFETs and Ge p-MOSFETs on Ge or Si platform, by taking the combined advantages of high electron mobility of GaAs and high hole mobility of Ge. However, despite their very similar lattice constants and thermal expansion coefficients, monolithic integration of GaAs and Ge remains challenging. Numerous technical issues need to be overcome in obtaining good quality GaAs epilayer on Ge, such as the polar-nonpolar nature, and distinct optimum growth temperature between GaAs and Ge. It has been shown that GaAs grown on vicinal Ge (100) substrates with 6° offcut toward (111) plane can eliminate the antiphase domain (APD) defects arises from their polar (GaAs)-nonpolar (Ge) nature.1,2 However, the large difference in optimum growth temperature for GaAs and Ge remains a challenge in GaAs–Ge monolithic integration due to atoms interdiffusion at the heterointerface.2–5 Most excellent quality GaAs can be obtained at 580 °C by molecular beam epitaxy and at 650 °C by metal organic chemical vapor deposition (MOCVD), much higher than the typical growth temperature for Ge at around 350–400 °C. Hence, GaAs grown at its optimum temperature on Ge will result in high Ge contamination, such as autodoping and formation of Ge-based complexes, as significant Ge atoms will diffuse into the GaAs epilayer during growth. On the other hand, growing GaAs at low temperature to prevent the outdiffusion of Ge atoms will be trade off with high arsenic-antisite defects in GaAs. Both of these growth conditions cannot provide satisfactory results. A usual approach to countermeasure this problem is to grow a low temperature GaAs buffer layer on Ge with thickness of about 100–200 nm before ramping up the growth temperature to that of the GaAs. This technique, however, does not reduce the diffusion length of As into the Ge substrate as demonstrated by Knuttilla et al.6 Kawai et al.6 suggested that the interdiffusion of the compositional atoms can be suppressed by applying a 30 nm AlAs initial layer in the GaAs-on-Ge system using 2° offcut Ge(111) substrates. However, substantial compositional diffusion of Al and Ge atoms into the GaAs epilayer was observed for samples grown at temperatures of >540 °C, before reaching the optimum growth temperature for GaAs. It is highly desirable to grow GaAs at its optimum temperature to ensure good structural and optical qualities for device applications. Also, for practical device applications, a conventional (100) substrate orientation is preferred. In this work, we present a detailed study on a series of GaAs/AlAs/Ge(100) samples with various AlAs interfacial layer thicknesses to examine the effectiveness of the AlAs layer in blocking the outdiffusion of Ge atoms into the GaAs epilayer at a high growth temperature of 650 °C by using MOCVD technique.

Four GaAs/AlAs/Ge(100) samples, with AlAs interfacial layer thicknesses of 0, 10, 20, and 30 nm were grown at 650 °C by using MOCVD technique. Vicinal Ge(100) substrates with 6° offcut toward the (111) plane were used to ensure that the GaAs epilayer grown on Ge is free from APD defects.2 Prior to the growth of AlAs and GaAs layers, Ge substrate was heated up to and kept at 650 °C for 5 min to remove the native oxide layer under H2 environment in the absence of As. Then tertiarybutylarsine and trimethylaluminum (TMAI) were introduced into the reactor for the growth of AlAs interfacial layer. Finally, by switching TMAI to trimethylgallium (TMGa), a 580 nm GaAs layer was grown at 0.32 nm/s. All layers were grown at a V/III ratio of 30.

Figure 1 depicts the transmission electron microscopy (TEM) images of the GaAs/AlAs/Ge samples. The actual AlAs thicknesses determined from TEM were 0, 9.5, 20, and 29 nm, in good agreement with the nominal values. High resolution TEM confirmed that the epilayers are free from APD defects. The corresponding secondary ion mass spectrometry (SIMS) profiles are shown in Fig. 2. For sample without the AlAs interfacial layer, Ge atoms outdiffuse up to

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300 nm into the GaAs epilayer, in good agreement with the results reported by Hudait and Krupanidhi. In contrast with the results reported by Kawai et al., where the diffusion of both Al (from a 30 nm AlAs layer on Ge substrate) and Ge atoms into the GaAs layer are substantial at a growth temperature of 600 °C, our SIMS results for samples with the AlAs interfacial layer show abrupt heterointerfaces and no significant compositional diffusion of Al and Ge atoms into the GaAs epilayer is observed at a high growth temperature of 650 °C. It was found that the Ge diffusion is completely blocked by the AlAs layer and no Ge atoms are able to penetrate into the GaAs layer, attributed to the higher Al–As bonding energy. The discrepancies between our results with those reported by Kawai et al. is possibly due to the different substrate orientations and offcut angles used. It has been shown that the best GaAs surface morphology was obtained from a 6° offcut Ge substrate, as compared to 2° and 9° offcut Ge substrates. Another notable difference between samples with and without AlAs interfacial layer is the diffusion of Ga and As atoms into the Ge substrate. Knuuttila et al. reported diffusion lengths of As into Ge for GaAs grown on Ge substrates at different growth temperatures, where As diffusion into Ge was found to be substantial even with the introduction of a low temperature (530 °C) grown GaAs buffer layer. This can be easily understood since As atoms will diffuse into the Ge substrate during the ramping up and at the high temperature (620 °C) growth of the GaAs layer, despite the existence of the preceding low temperature grown GaAs. In contrast, as shown in this work, with an AlAs interfacial layer, the diffusion of As atoms into Ge substrate is negligible at a high growth temperature of 650 °C.

For direct comparison, the Ge and As diffusion lengths for all the samples determined from SIMS measurements were plotted together in Figs. 3(a) and 3(b), respectively. As shown in Fig. 3(a), the diffusion length of the Ge atoms in sample without the AlAs interfacial layer is about six times longer than those samples with AlAs. Close examination on the Ge diffusion profiles for various AlAs interfacial layer thicknesses show subtle differences after the Ge intensity (concentration) dropped below 25% of its original value ($I_o$), the Ge diffusion into AlAs layer marginally increases with increasing AlAs thickness. As all the samples were grown at the same temperature of 650 °C, these differences are strong evident of Ge atoms segregation during AlAs growth.

![FIG. 1. TEM images of the GaAs/AlAs/Ge samples suggest the GaAs and AlAs thicknesses were (a) 586 and 0 nm, (b) 568 and 9.5 nm, (c) 564 and 20 nm and (d) 590 and 29 nm, respectively.](image1)

![FIG. 2. (Color online) SIMS profiles for GaAs/AlAs/Ge samples with AlAs nominal thickness of (a) 0, (b) 10, (c) 20, and (d) 30 nm. The corresponding TEM image for each sample is placed behind the graph to illustrate the position of the layers.](image2)
evidenced in Fig. 3(b), the diffusion of As atoms into the Ge substrate has reduced about four times from 100 to 25 nm with the presence of the high atomic bonding energy AlAs interfacial layer. Our results suggest that the thickness of the AlAs interfacial layer can be reduced to 10 nm without affecting its effectiveness in blocking the cross diffusion of Ge, Ga, and As atoms between the GaAs layer and Ge substrate.

Shown in Fig. 4 are the room temperature photoluminescence (PL) for samples with (solid line) and without (dotted line) AlAs interfacial layer, measured using a 532 nm laser at an excitation power of 5 mW. For sample without the AlAs interfacial layer, a broad inner-bandgap emission at 900–1200 nm observed beside the main peak at 860 nm corresponds to the GaAs bandgap at room temperature. This broad emission is likely caused by the Ge-based complexes formed inside the GaAs layer. All other samples with AlAs interfacial layer show a single peak PL emission, suggesting that the Ge diffusion into the GaAs layer is negligible, in corroborations with SIMS results.

In summary, a series of GaAs/AlAs/Ge(100) samples with AlAs interfacial layer thicknesses of 0, 10, 20 and 30 nm were grown at 650 °C and characterized by TEM, SIMS, and PL techniques. Our results suggest that AlAs interfacial layer as thin as 10 nm is sufficient to effectively block the outdiffusion of Ge atoms at a high growth temperature of 650 °C, eliminating Ge-based complexes and autodoping effects in the GaAs layer. In corroborations with SIMS results, PL measurements confirmed that Ge diffusion into the GaAs layer is negligible where no emission from GaAs-based complexes at 900–1200 nm is observed. The insertion of an AlAs interfacial layer is a cost-effective way to solve the incompatibility in growth temperature for GaAs on Ge substrates, avoiding wasteful thick buffer layer and ensuring high purity GaAs by eliminating cross diffusion of Ge, Ga, and As atoms at the heterointerface.

The authors would like to thank Debbie H. L. Seng for her assistance in SIMS measurements.


FIG. 3. (Color online) Comparison of (a) Ge and (b) As diffusion lengths for samples with different AlAs interfacial layer thicknesses. Dot-dashed line: AlAs=0 nm, broken line: AlAs=10 nm, solid line: AlAs=20 nm, and dotted line: AlAs=30 nm. All samples were grown at a substrate temperature of 650 °C.

FIG. 4. (Color online) Room temperature PL for samples with (solid line) and without (dotted line) AlAs interfacial layer. No emission at 900–1200 nm due to Ge-based complexes is observed from samples with AlAs interfacial layer.