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Reducing threading dislocation density in GaSb photovoltaic devices on GaAs by using AlSb dislocation filtering layers

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ABSTRACT

GaSb based photovoltaic devices have been demonstrated on GaAs substrates by inducing interfacial array of 90° misfit dislocations. Despite the beneficial qualities of the highly stable 90° misfit dislocation, there is a significant density of residual threading dislocations in the GaSb layer, resulting in the degradation of the electrical performance of such photovoltaic cells compared to lattice matched devices. We aim to reduce threading dislocation density by optimizing growth temperature and by using an AlSb dislocation filtering layer. The growth temperature optimization results in a reduction of the threading dislocation density to 1.3×10^8 cm^{-2}. Adding an AlSb dislocation filtering layer further improves the electrical performance of the GaSb solar cells by reducing the threading dislocation density to 4×10^7 cm^{-2}. A comparison between the experimental data and theoretical calculation confirms that the recombination in dislocation centers is a dominant loss mechanism in GaSb solar cell grown on GaAs substrate.

1. Introduction

To date, multijunction solar cells (MJSC) are the most efficient photovoltaic devices to convert solar energy into electrical power [1]. These devices consist of several solar cells monolithically stacked from high to low bandgaps which allows for the absorption of distinct spectral bands, thereby reducing the thermalization losses incurred by the absorption of high energy photons in low bandgap semiconductors. Also, unlike single junction cells such as those based on silicon, in multijunction cells, using near IR narrow bandgap subcells reduces the loss associated with un-absorbed low energy photons [2]. MJSCs have however typically been limited to lattice matched systems which are highly restricted in terms of the availability of semiconductor materials with required bandgaps. Mechanically stacking two or more MJSCs can resolve this issue and have resulted in record efficiencies [3,4]. However, using the mechanically stacked MJSC approach increases the cost of production and also adds fabrication complexity. The restrictions imposed by high cost and lack of availability of lattice matched materials have resulted in exploration of lattice mismatched or more specifically, metamorphic photovoltaic devices.

GaAs is a very suitable substrate for use in MJSCs. There are many high efficiency GaAs based dual and triple junction solar cells reported in the literature [5,6]. The top junction material, such as InGaP or AlGaAs, is grown lattice matched to GaAs. There is however an issue with the lack of lattice matched narrow bandgap materials on GaAs to be used as a narrow bandgap absorber for NIR part of the spectrum. This can be addressed by using a metamorphic layer such as InGaAs as the bottom junction. Geisz et al. have reported 33.8% efficiency for a triple junction solar cell using $In_{0.3}Ga_{0.7}As$ (1.0 eV) with 2% lattice mismatch to GaAs as the bottom junction of the GaAs/InGaP solar cell [7]. The addition of such metamorphic layers leads to a high threading dislocation density (TDD) in the InGaAs layers and epitaxial strategies involving step-graded buffer layer have been employed to possibly reduce the formation of such dislocations [8,9]. Using buffers adds significant complexity to the growth of the solar cells, these epitaxial layers typically have a finite residual strain in them due to partial relaxation, thus making it very difficult to reproducibly grow solar cells on them.

An alternative method to realize a narrow bandgap subcell on GaAs is to grow GaSb on it through the realization of interfacial misfit dislocation arrays (IMF) [10–12]. The growth of GaSb on GaAs has been shown to start off as islands and later coalesce into a uniform layer. At the interface, the strain energy is relieved by both 90° and 60° misfit dislocations. While most of the strain is believed to be relieved by the laterally propagating 90° misfit dislocations, the minority 60° dislocations end up causing threading dislocations in the GaSb epitaxial layer.

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The formation of the 60° dislocations has been traced back to the point of coalescence of the GaSb islands, where two arrays of periodic misfit dislocation arrays meet [13]. The fundamental approach behind the IMF technique is to minimize these points of coalescence by inducing the periodic dislocation arrays over as large an area as possible [14]. However, if the conditions for the formation of the IMF (explained later) are not fully optimized, there will be a very high island density and the GaSb in turn will have a high TDD ($> 10^{10}$ cm^{-2}). Therefore, it is critical to understand the effect of parameters such as nucleation temperature, growth sequence and III:V ratio on the epitaxial process [15,16].

In this study, we focus on the fabrication of GaSb photovoltaic devices on GaAs by reducing the TDD involved in the IMF technique. We achieve this by optimizing the growth temperature and by using an AlSb layer as a dislocation filtering layer (DFL). The evidence for the formation of the IMF array is provided by a detailed transmission electron microscopy (TEM) analysis of the interface. The TDDs are independently calculated using cross-section TEM and plan-view TEM images. The TDD values are extracted from the plan view TEM images, while the cross-section images are used to observe the propagation and bending of threading dislocation in the layers. Finally, the solar cell parameters such as open circuit voltage and short circuit current density are modeled for various densities of threading dislocations and the electrical performance of the GaSb IMF grown solar cell on GaAs substrates are presented.

2. IMF growth temperature optimization

The epitaxial samples used in this study were grown on GaAs (001) substrates in a VG V80 solid source molecular beam epitaxy (MBE) reactor. The substrate temperature is measured using an optical pyrometer. The oxide on the GaAs substrate is desorbed at 630 °C for 20 min before a 200 nm GaAs smoothing layer is grown at 580 °C. At this point, the arsenic cracker is valved off to initiate the desorption of arsenic from the surface. The reflection high-energy electron diffraction (RHEED) pattern transforms from a (2 × 4) As-stabilized GaAs surface to a (4 × 2) Ga-rich surface. Following this, the sample is exposed to an antimony flux and the RHEED pattern changes to a (2 × 8) reconstruction. As shown by Huang et al., this interaction of Sb_2 with a Ga-rich surface is critical to forming the IMF [17]. Once the (2 × 8) reconstruction is observed, the substrate temperature is brought down to the growth temperature of GaSb under Sb_2 overpressure and the growth is initiated.

For this study, four different 2 µm thick GaSb layers are grown at 420, 460, 500 and 540 °C. Within the first few monolayers of GaSb growth, the RHEED shows a (1 × 3) reconstruction surface. A constant V/III ratio of 1.5:1 is maintained between Sb and Ga across all samples. Also, the GaSb growth rate (calibrated by RHEED oscillations) is kept constant at 0.3 ML/sec.

The bright-field cross-sectional TEM images along [110] direction of the 2 µm thick IMF grown GaSb epilayers at different growth temperatures (420, 460, 500 and 540 °C) are shown in Fig. 1(a)-(d). At a higher magnification (Fig. 1(e) & (f)), all samples show a highly periodic array of misfit dislocations at the GaAs/GaSb interface confirming the formation of the IMF. It can clearly be seen from Fig. 1, that at a higher growth temperature (540 °C) the initial growth conditions for GaSb aren't optimized and TDD formation at the interface is higher. As demonstrated before [18], it can be seen that the TDD dramatically decreases with increase in the film thickness due to mutual interactions between dislocations at all growth temperatures. Using the projected length of dislocation lines in a TEM image, the threading dislocation density can be estimated by the following equation: [19]

$$TDD = \frac{4}{\pi}\frac{l'}{At} \tag{1}$$

where t is the thickness of the sample and A is the area over which the projected length l' is estimated. From Fig. 1(a)-(d), the TDD is estimated using Eq. (1) at different temperatures within the first 0.5 µm GaSb layer. The projected length l' is measured using the appropriate scale. While the dislocation density is estimated to be $\sim 5.6 \times 10^8$ cm^{-2} for the sample grown at 540 °C, there is a decrease in the TDD to 1.5×10^8 cm^{-2} at a growth temperature of 420 °C. Plan-view TEM images (Fig. 2) of the GaSb surfaces grown at different temperatures (540, 500, 460, and 420 °C) are analyzed to verify the TDD obtained. As observed by cross-sectional TEM, a similar trend in the dislocation density can be seen from plan-view TEM images in Fig. 2, with the sample grown at a higher growth temperature showing a higher TDD. Analyzing a typical 3 µm^2 surface by directly counting the number of dislocations, the TDD from the plan-view images could be estimated to be 5.9×10^8 cm^{-2} for GaSb surface grown at 540 °C and again decreases to $\sim 1.3 \times 10^8$ cm^{-2} for the sample grown at 420 °C. While the plan-view TEM images are more accurate in TDD calculations, the cross-section images show us both the quality of the IMF layer and the progression of the threading dislocations through the epitaxial structure.

For characterization of the strain relaxation using High Resolution X-ray Diffraction (HRXRD), conventional triple crystal ω–2θ scans were conducted in the vicinity of symmetrical (004) reflection. Two peaks - one from the GaAs substrate and the other from GaSb (004) - are seen in each curve (not shown here). The peak position of GaSb relative to the substrate was nearly identical for all growth temperatures. However, the FWHM of the epi layer grown at 420 °C is lowest and equal to 120 arcsecs, which indicates a higher crystal quality. Also, to visualize the angle distribution of coherent and diffused scattered x-ray radiation and evaluation of residual elastic stress and extent of relaxation, triple crystal ω–2θ/ω reciprocal space maps (RSM) were measured in the vicinity of the symmetrical and asymmetrical reflections. Fig. 3 shows the RSM for the sample grown at 460 °C in < 004 > and < 224 > directions. From the RSM, we can see that there is no tilt in the epilayer with respect to the substrate along the completely strain-relaxed [224] line. The lattice misfit relaxation for samples grown at all temperatures are calculated to be in the range of 99.5–100%. This indicates that the GaSb growth temperature doesn't necessarily affect the relaxation of the GaSb bulk layer.

3. AlSb dislocation filtering layer

Use of dislocation filtering layer (DFL) in lattice mismatched epitaxial growth is one strategy for reducing unwanted threading dislocation. Matthews et al. published a report detailing the mechanism by which dislocations will bend at an interface [20]. Many examples of DFLs can be found in literature such as the use of GaAsP/GaAs strained superlattices to filter dislocation formed in GaAs epitaxial layers grown on Si [21] and the use of quantum dots layers as dislocation bending sites to filter dislocations in GaAs-based laser on Si [22,23].

In the case of the GaSb/GaAs system, Qian et al. introduced buffer layers of AlSb, InGaSb, and an AlSb/GaSb strained superlattices (SLS) at the GaAs interface and measured the associated reduction in TDD for the subsequent GaSb growth [18]. There are several publications that make use of an AlSb nucleation layer and AlSb/GaSb SLS to improve the quality of GaSb epilayer on top of GaAs [24–26]. There is also an added advantage of using AlSb layers directly on GaAs substrates. Ripalda et al. have made use of metamorphic AlSb layers on GaAs to create a compliant substrate on which strain free GaSb can be grown [27]. However, growing AlSb directly on GaAs has not resulted in the same TDD reduction that we are able to achieve by growing GaSb on GaAs. However, adding an AlSb layer as a defect filter has shown significant promise. In the following paragraph we study the effect of an AlSb DFL layer's position with respect to the IMF array on the TDD in GaSb epilayers.

In our study, three samples with AlSb DFLs were grown on GaAs. DFLs were placed at distances of 100 nm, 250 nm, and 500 nm from the GaSb/GaAs interface. The AlSb DFL layers were grown 250 nm thick.