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Study of the Growth and Dislocation Blocking Mechanisms in $\text{In}_x\text{Ga}_{1-x}\text{As}$ Buffer Layer for Growing High-Quality $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$, $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$, and $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ on Misoriented GaAs Substrate for Inverted Metamorphic Multijunction Solar Cell Application

Abstract: Effects of growth conditions and buffer structures on crystal quality of 1.9-eV $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$, 1-eV $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$, and 0.75-eV $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ materials on misoriented GaAs substrate for inverted metamorphic solar cell grown by metalorganic chemical vapor deposition have been studied. Large lattice mismatch issue between the two lower bandgap 1.0-eV $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ and 0.75-eV $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ epilayers and the substrate has been resolved by using optimized step-graded buffer layers. Threading dislocation blocking mechanisms have been studied and discussed. It was indicated that threading dislocations have been significantly blocked in the designed InGaAs buffer layers through annihilation reactions between threading dislocations or through the formation of misfit dislocations. As a result, smooth surface $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ and $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ epilayers with threading dislocation density of about $1 \times 10^6 \text{ cm}^{-2}$ were obtained. For the growth of InGaP, the surface morphology, crystal quality, ordering parameter, and InGaP composition were significantly affected by growth temperature, V/III ratio, and III/III ratio. The almost lattice match to the substrate, high crystal quality, and smooth surface of $\text{In}_{0.495}\text{Ga}_{0.505}\text{P}$ were obtained at growth temperature of 675°C and V/III ratio above 150. The ordering parameter was strongly

dependent on growth temperature. Photoluminescence measurement indicated that the bandgap of the InGaP epilayer is 1.89 eV, indicating that the solid composition in the InGaP film is more disordered.

Keywords: InGaAs, InGaP, IMM, solar cell, MOCVD, threading dislocation, misorientation substrate

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1 Introduction

In the past year, researchers have reported record-breaking conventional 3-junction solar cells with conversion efficiencies of up to 41.6% (King et al. 2012), and scientists are now looking at overcoming the next performance barrier of 50% (Leite et al. 2013). Despite the high efficiency, it is well known that the 3-junction cell bandgap combination compromises the ideal solar spectrum splitting in favor of subcell material quality, hence limiting the achievable efficiency. Current match for such cells is a major constraint for further improvement of efficiencies. Future terrestrial cells will likely feature four or more junctions with performance potential capable of reaching over 50% efficiency at concentration (Law et al. 2010). The 4-, 5-, or 6-junction concentrator cells trade lower current densities for higher voltage and divide the solar spectrum more efficiently. For example, theoretical calculations indicate an ideal efficiency of over 59% for a 4-junction cell with bandgap combination of 1.9/1.42/1.02/0.75 eV (Law et al. 2010). In these designs, III/V materials which have energy bandgap about 1.0–1.05 and 0.7–0.75 eV play very

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important roles (Sherif et al. 2005). InGaAs seems to be the best choice of material for this range of bandgap. However, the 2.4% and 4% lattice mismatch between 1.0-eV $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ and 0.75-eV $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ and GaAs substrates, respectively, imposes difficulty to grow high-quality material. It is thus more challenging and even more difficult to grow a high bandgap subcell above it. In recent years, researchers have tried to apply advance technologies including metamorphic growth on Ge (King et al. 2007), novel lattice-matched designs (Green et al. 2013), inverted metamorphic (IMM) growth (Geisz et al. 2007), or wafer bonding technique (Bett et al. 2013) to increase the efficiency of solar cell. Table 1 summarizes recent results of III/V solar cell performance and material growth for solar cell application. Although 4-junction solar cell using wafer bonding technique has achieved new record efficiency of 44.7% (AM1.5D, 297 suns), the structure, however, consists of two dual junctions GaInP/GaAs and GaInAsP/GaInAs grown on two expensive GaAs and InP substrates, which may result in high production cost (Bett et al. 2013). IMM growth solution has been developed to overcome the current matching and lattice-mismatch issues in multijunction cells, and 40.8% (AM1.5D, 326 suns) efficiency of 3J-IMM $\text{In}_{0.49}\text{Ga}_{0.51}\text{P}/\text{In}_{0.04}\text{Ga}_{0.96}\text{As}/\text{In}_{0.37}\text{Ga}_{0.63}\text{As}$ has been reported (Geisz et al. 2008). Similar to metamorphic growth, a graded InGaAs buffer layer is utilized to change the lattice constant of subsequent growth. However, in this

method the solar cell is grown upside down with the top cell InGaP, lattice matched to the substrate grown first, followed by the middle cell that is either GaAs or mismatched GaInAs grown lattice matched to the substrate. The bottom (most highly lattice mismatched) cells are grown last. By this approach, the top cells will be maintained as defect free, while limiting the defects from the buffer region into the lower cells which are not as easily affected as the top subcell. Additionally, Tatavari *et al.* have developed a full-wafer epitaxial liftoff technology that allows to separate the grown structure and expensive substrate (Tatavari et al. 2009). This advanced technology not only allows to reduce cell cost due to the possibility of substrate reuse multiple times but also to lower the total weight of IMM multijunction cells. A schematic 4-junction IMM solar cell structure is illustrated in Figure 1(a). Recently, an efficiency of 34.5% (AM0, 1 sun) for a 4-junction IMM has been achieved (Patel et al. 2012). However, the efficiency of the 4-junction IMM is still lower than prediction. The lower performance was likely attributed to high dislocation density, which causes degradation of the performance of device, in the subcells caused by large lattice mismatch between the subcells and substrate. Therefore, it is necessary to find out an effective method to block dislocations from propagating to active layers in such lattice-mismatched InGaAs/GaAs material for future multijunction IMM solar cell application.

Table 1 Summary of material growth and device performance of III/V compound solar cells

Reference				Material growth		Solar cell performance	
	Structure	Growth technique	Relaxation degree (%)	Surface roughness (nm)	TDD (cm^{-2})	V_{oc} (V)	Efficiency (%)
SpectroLab (King et al. 2007)	$\text{In}_{0.44}\text{Ga}_{0.56}\text{P}/\text{In}_{0.08}\text{Ga}_{0.92}\text{As}/\text{Ge}$	MM-MOCVD	100	–	–	2.911	40.7-AM1.5D under 240 suns
NREL (Green et al. 2013)	$\text{InGaP}/\text{GaAs}/\text{InGaAs}(\text{Sb})$	LM-MBE	99	–	–	–	43.5-AM1.5D under 360 suns
EMCORE (Patel et al. 2012)	$\text{In}_{0.5}\text{Ga}_{0.5}\text{P}/\text{GaAs}/\text{In}_{0.3}\text{Ga}_{0.7}\text{As}/\text{In}_{0.6}\text{Ga}_{0.4}\text{As}$	IMM-MOCVD	100	–	5×10^6	3.236	34.5-AM0 under 1 sun
Fraunhofer (Bett et al. 2013)	2J (GaInP/GaAs) + 2J (GaInAsP/GaInAs)	MOCVD	–	–	–	4.165	44.7-AM1.5D under 297.3 suns
N. J. Quitoriano (Quitoriano and Fitzgerald 2007)	$\text{In}_{0.54}\text{Ga}_{0.46}\text{As}/\text{GaAs}$	MM-MOCVD	99	15	3.1×10^7	–	–
K. E. Lee (Lee and Fitzgerald 2010)	$\text{In}_{0.42}\text{Ga}_{0.58}\text{As}/\text{GaAs}$	MM-MOCVD	86.9	4.8	3.6×10^7	–	–
G. B. Galiev (Galiev et al. 2014)	$\text{In}_{0.64}\text{Ga}_{0.36}\text{As}/\text{GaAs}$	MM-MBE	95	6	5×10^6	–	–

Notes: MM: metamorphic; LM: lattice-matched; IMM: inverted metamorphic; MBE: Molecular Beam Epitaxy.

Figure 1 (color online). (a) Schematic 4-junction IMM solar cell. (b) Designed $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer profiles using 6-, 8-, and 10-SG buffer layer for growing $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ on GaAs substrate

In previous work, the effects of different substrate misorientation degrees and growth temperature on material properties of the $n^{++}\text{-GaAs}/p^{++}\text{-AlGaAs}$ tunneling diode and crystal quality of the $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ layer have been investigated. It is found that the misorientation influences both surface roughness and interface properties of the $n^{++}\text{-GaAs}/p^{++}\text{-AlGaAs}$ tunneling diode. The use of 10° offcut GaAs substrates resulted in reducing oxygen contamination in $n^{++}\text{-GaAs}$ and $p^{++}\text{-AlGaAs}$ layers due to the reduction of sticking coefficient and number of anisotropic sites (Yu et al. 2010). Moreover, the effect of GaAs substrate misorientation on surface morphology and crystal quality of 1-eV $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ was affected by the growth mode by changes in surface free energy and also by the formation, gliding, and multiplication of dislocations (Nguyen et al. 2011). The work indicated that a better crystal quality $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ layer with threading dislocation (TD) density as low as $1 \times 10^6 \text{ cm}^{-2}$ has been achieved on a 6° offcut substrate using a 10-step-grade (SG) buffer layer. However, the buffer layer thickness of $1.5 \mu\text{m}$ seems to be quite thick for IMM solar cell application.

This paper reports more detailed experimental results on $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ and 1.0- and 0.75-eV $\text{In}_x\text{Ga}_{1-x}\text{As}$ for 4 or more junction IMM solar cell application. For InGaP, the experiment aims at optimization of growth conditions for achieving high crystal quality, smooth surface InGaP, which provides better conditions for growing subcells on top. For InGaAs subcell growth, TD blocking mechanisms and buffer structure are studied in detail for reducing TD density in the subcells to about 10^6 cm^{-2} .

2 Experiment methods

In the experiment, InGaP and InGaAs samples were grown on epi-ready GaAs (001) substrates with 6° offcut toward [110] direction. Metalorganic chemical vapor deposition (MOCVD-EMCORE D180) was used to grow the epilayers. Group-III precursors of trimethylindium and trimethylgallium and group-V precursor of pure arsine (AsH_3) and phosphine (PH_3) were used. The indium composition and degree of relaxation were determined with a high-resolution X-ray diffractometer (HR-XRD). The surface texture and roughness were examined by atomic force microscopy (AFM). The dislocation densities were characterized by cross-sectional and plan-view transmission electron microscopy (TEM). The bandgap of InGaP was determined using photoluminescence (PL) performed at room temperature.

3 Results and discussion

3.1 The growth of $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ cell on GaAs substrate

Due to high cracking temperature of PH_3 source, InGaP compound normally is grown at high temperature. Moreover, difference in bond dissociation energy between InP (46.8 kcal/mol) and GaP (58.4 kcal/mol) (Seki, Watanabe, and Matsui 1978), and As and P intermixing may form unnecessary phase at interface between InGaP

and GaAs and degrade InGaP quality. Therefore, any change in growth conditions such as growth temperature, V/III ratio, partial pressure, and $\text{III}_{(\text{In})}/\text{III}_{(\text{Ga})}$ may result in different InGaP composition and its crystal quality. Our experimental results show that better crystal quality and smoother surface $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ epilayer was obtained at growth temperature of 675°C and high V/III ratio conditions. As shown in Figure 2(a), the best surface roughness of 0.8 nm was obtained on the sample grown at a temperature of 675°C and V/III ratio of above 150. With the smooth surface InGaP having been achieved, we believe that the further growth of 1.42-eV GaAs mid-cell and other components of IMM structure on top of InGaP will not be affected. The sample also exhibited good interface between InGaP and GaAs substrate as illustrated in Figure 2(b). Lower or higher growth temperature causes worse crystal quality and rougher surface roughness. The reason is that the PH_3 cracking efficiency was too low at lower growth temperature causing insufficient phosphorus for InGaP formation. On the other hand, higher growth temperature will increase the desorption rate from surface for In atoms compared to Ga atoms (Hageman et al. 1992). The lack of In during the solidification process will, therefore, affect the crystal quality due to larger lattice mismatch between the epilayer and substrate.

InGaP is lattice matched to GaAs at the Ga content of 51%. A varied composition would cause a tensile or compressive stress that degrades the crystal quality of the InGaP epilayer. Figure 2(c) shows (004) ω - 2θ XRD pattern of InGaP epilayer grown on GaAs substrate at 675°C using two different $\text{III}_{(\text{In})}/\text{III}_{(\text{Ga})}$ ratios. It is seen that almost lattice match and smooth surface InGaP on GaAs substrate can be attained in the range of $\text{III}_{(\text{In})}/\text{III}_{(\text{Ga})}$ ratio of 1.69–1.81 at the same growth condition. Any change in $\text{III}_{(\text{In})}/\text{III}_{(\text{Ga})}$ ratio far from this range would result in higher mismatch that causes an increase in the surface roughness of the epilayer. Figure 2(d) shows the PL spectra of the $\text{In}_{0.495}\text{Ga}_{0.505}\text{As}$ layer measured at room temperature. The layer exhibited PL main peak at 656 nm with the full width half maximum value of 17 meV. The bandgap of the epilayer, therefore, was derived from PL peak position to be 1.89 eV. The ordering parameter of 0.48 calculated based on the method developed by Murata, Ho, and Stringfellow (1997) suggested that Ga and In atoms in the InGaP film tend to arrange more randomly. However, it was found that the degree of ordering parameter was increased with increasing growth temperature, suggesting that the bandgap of $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ could be tuned just by tuning degree of ordering through changing growth temperature (Zunger and Mahajan 1994), V/III ratio, surfactant treatment (Mori and

Figure 2 (color online). (a) AFM image, (b) cross-sectional TEM, (c) (004) ω - 2θ scan XRD, and (d) PL spectra measured at room temperature of $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ grown on GaAs at 675°C and V/III ratio of 150–180

Fitzgerald 2009), or strain in the epilayer (Novak et al. 2002; Garcia et al. 2008).

3.2 TD blocked in optimized step-graded $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer for growing high crystal quality 1-eV and 0.75-eV InGaAs

We first study the gliding and blocking process in $\text{In}_x\text{Ga}_{1-x}\text{As}$ SG buffer layer for the purpose of growth high crystal quality 1.0-eV $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ on GaAs substrate. For the purpose of study, three samples were grown using three different buffer structures as shown schematically in Figure 1(b). In the three samples, buffer layers including 6, 8, and 10 individual SG $\text{In}_x\text{Ga}_{1-x}\text{As}$ layers with different composition gradients and/or starting indium concentration values at the interface were grown first, before the fixed composition $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayers were grown on the top. In the three buffer structures, the thickness of individual layer in the buffer layer was grown exceeding the critical thickness because it is believed that TD density can be reduced through reaction with other TDs or blocked by misfit dislocations (MDs) during the strain relaxation in metamorphic structure (Romanov et al. 1999). Modeling study (Speck et al. 1996) suggested that the use of multiple discrete strained layers, which were grown over their critical thickness, can provide a marked reduction in TD density through annihilation reactions and blocking process (Freund 1990). The critical thickness of individual layer was estimated based on Matthews-Blakeslee model (Matthews and Blakeslee 1974) as stated in eq. [1]:

$$h_c = \frac{|b|}{8\pi\epsilon_m \cos \lambda} \left(\frac{1 - \nu \cos^2 \beta}{1 + \nu} \right) \ln \left(\frac{ah_c}{|b|} \right). \quad [1]$$

Equation [1] can be simplified to $h_c \approx |b|/\epsilon_m$ because the product of all the other terms in the equation are approximately constant and have magnitude on the order of one, where $|b|$ is the magnitude of Burgers vector b , and ϵ_m is misfit strain.

Figure 3(a)–3(c) shows the cross-sectional bright-field TEM images of the three samples grown using 6-, 8-, and 10-SG $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers, respectively. Although some TDs have been blocked in the buffer layer for the 600-nm-thick 6-SG InGaAs grade buffer, some TDs, however, still propagate into the fixed composition epilayer and end at the free surface (see cross-sectional TEM micrograph in Figure 3(a)), resulting in higher TD density of about $7 \times 10^6 \text{ cm}^{-2}$, as indicated by plan-view TEM micrograph in Figure 5(b). TDs extended from the bottom and higher misfit strain in the 6-SG buffer layer have worsened the surface morphology of the top surface layer. AFM study (Figure 4(a)) shows the surface morphology with root mean square (RMS) roughness of 2.7 nm for the 6-SG InGaAs buffer. Interestingly, the 8-SG and 10-SG buffer layers, although greater in thickness (1 and 1.5 μm , respectively), showed no obvious TD in the fixed composition $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ layer as shown in the plan-view TEM image of Figure 3(b) and 3(c), respectively. It is clear that TDs were blocked and contained within the buffer layers, resulting in almost no TDs extension into the $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayer. Better surface roughness was also observed on the two samples as shown in Figure 4(b) and 4(c). Surface roughness with RMS value of 1.8 and 1.5 nm for samples using 8-SG and 10-SG, respectively, were obtained. The lower TD densities in the epilayers were attributed to the lower misfit strain between individual buffer layer and more discrete strained layers in 8- and 10-SG buffer structure. It has been reported that in lattice-mismatched zinc blend crystal, with low misfit strain, strain relaxation occurs primarily by the formation of $60^\circ a/2 \{110\}\{111\}$ misfit dislocations (Speck et al. 1996). At the end of every MD, TD segments are generated and often find their way into the active layer (Goldman et al. 1998). If TDs are glissile, then for [001] growth they will glide in one of four {111} slip planes. Thus, there are four unique {111} planes and six unique (110) directions. Considering that the dislocation Burgers vectors can assume either positive or negative sense, there are 12 possible Burgers vectors. Finally, a

Figure 3 (a)–(c) Cross-sectional bright-field TEM images of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ film grown on GaAs substrate using 6-, 8-, and 10-SG $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers, respectively

Figure 4 (Color online). (a)–(c) AFM images of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayers grown on GaAs substrate using 6-, 8-, and 10-SG $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers, respectively

glissile dislocation with an $a/2 \langle 110 \rangle$ Burgers vector can have its line in one of two possible $\{111\}$ planes and thus there are a total of 24 specific dislocation Burgers vector/slip plane combinations (Speck et al. 1996). In all possible combinations between TDs, only certain TDs which have antiparallel Burgers vector can fall into annihilation reactions, the remaining combinations may result in new TD segments through fusion reactions and these new TD segments tend to move up to active layer. Therefore, the purpose of multiple discrete layers in metamorphic growth is to increase the probability of annihilation reactions between TDs. As can be seen in Figure 3(b) and 3(c), both annihilation and fusion reactions between TDs in the buffers were observed. Simultaneously, mobile TD blocked by MD process was also observed. Figure 5(a) presents a plan-view TEM image observed at two $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer interface showing a number of dislocation intersection events. It is observed that when dislocation intersections occur, a variety of interactions can take place. As marked at points B and C, where two pairs of $a/2 \langle 110 \rangle$ MDs fell into interaction, no blocking interaction happened, their TD arms still glided up on their $\{111\}$ glide planes. However, at point A, the motion of TD arm was blocked. We believed that TD blocking processes observed from TEM images explain for better crystal quality in the $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayers grown using 8- and 10-SG buffer layers. Figure 5(c) shows plan-view TEM image of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ on 8-SG sample, only one TD

appeared indicated by the circle marked in the figure, indicating that a TD density of about $1 \times 10^6 \text{ cm}^{-2}$ in the $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayer has been obtained.

After optimizing the thickness and composition profile of $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layer for growing high crystal quality 1-eV subcell, we continued growing a “quasi-structure” of 2-junction 1- and 0.75-eV subcell on GaAs substrate. The structure includes $3 \mu\text{m}$ $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ on 8-SG $\text{In}_x\text{Ga}_{1-x}\text{As}$ ($x = 0.05\text{--}0.3$) followed by $0.8 \mu\text{m}$ 6-SG $\text{In}_x\text{Ga}_{1-x}\text{As}$ ($x = 0.35\text{--}0.5$) buffer layer, concluded by the growth of final $1.5 \mu\text{m}$ $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ epilayer. Interestingly, the crystal quality of 1-eV $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ was not affected by the growth of subsequent InGaAs buffer layer and 0.75-eV $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ epilayer. As shown in Figure 6(a), no TD was observed in the $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ and $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayers. The plan-view TEM image (Figure 6(b)) of the $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ epilayer shows only three TDs (appearing near stars masked in the figure) on a large area of $200 \mu\text{m}^2$, which corresponds to a TD density of $1.5 \times 10^6 \text{ cm}^{-2}$ in $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$. The growth of high indium composition also caused an increase in RMS roughness of the film to 2.4 nm (Figure 6(c)).

Figure 6(d) represents the asymmetric scan for (115) reflection obtained from 1.5 and $3 \mu\text{m}$ $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ and $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayers on GaAs substrate, respectively. Asymmetric rocking curve scans on (115) reflection of substrate were recorded in $\omega\text{--}2\theta$ scans to determine indium composition and relaxation degree of $\text{In}_x\text{Ga}_{1-x}\text{As}$

Figure 5 (a) Plan-view TEM image observed at the interface between two $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers in 8-SG buffer structure. (b) Plan-view TEM image of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ epilayer on GaAs substrate using 6-SG, and (c) 8-SG buffer layer

Figure 6 (Color online). (a) Cross-sectional TEM image, (b) plan-view TEM image, (c) AFM image, and (d) (115) ω - 2θ scan XRD of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ and $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ epilayers grown on GaAs substrate by optimizing the $\text{In}_x\text{Ga}_{1-x}\text{As}$ buffer layers

alloy on GaAs substrate. The indium composition (x) in $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayer is obtained using Vegard's law (Bowen and Tanner 2005)

$$x = \frac{a_f - a_s}{a_{\text{InAs}} - a_s}, \quad [2]$$

where $a_s = 5.6533 \text{ \AA}$, $a_{\text{InAs}} = 6.0583 \text{ \AA}$ are lattice constants of GaAs substrate and InAs, respectively. a_f is bulk equivalent or unstrained lattice constant defined by

$$a_f = \frac{a_{\perp} - 2a_{\parallel}(\frac{\nu}{1-\nu})}{1 - 2(\frac{\nu}{1-\nu})}, \quad [3]$$

where ν is Poisson ratio, $a_{\parallel}$ and $a_{\perp}$ are the in-plane and out-of-plane lattice parameters of $\text{In}_x\text{Ga}_{1-x}\text{As}$ epilayers, respectively, calculated from Bragg's law reflection position by

$$a_{\parallel} = \frac{\lambda \sqrt{h^2 + k^2}}{2 \sin \theta_B \sin \phi}; \quad a_{\perp} = \frac{\lambda l}{2 \sin \theta_B \cos \phi}, \quad [4]$$

where θ_B is Bragg angle, ϕ is the angle between the diffraction plane and the sample surface, h , k , and l are Miller indices of reflection plane, and λ is the wavelength of the X-rays ($\lambda = 1.5406 \text{ \AA}$). Degree of relaxation R is defined by

$$R = \frac{a_{\parallel} - a_s}{a_f - a_s} 100\%. \quad [5]$$

Bragg angles were determined from peak position of $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ and $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$ epilayers, and the in-plane and out-of-plane lattice parameters were calculated to respective values $a_{\parallel} = 5.7625 (\pm 0.001) \text{ \AA}$, $a_{\perp} = 5.7836 (\pm 0.001) \text{ \AA}$ for $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$, and $a_{\parallel} = 5.8651 (\pm 0.001) \text{ \AA}$ and $a_{\perp} = 5.8705 (\pm 0.001) \text{ \AA}$ for $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$. From [2] and [6], the indium composition and relaxation degree of the epilayers were defined as $x = 0.295 \pm 0.05$ and $R = 91\%$ for $\text{In}_{0.3}\text{Ga}_{0.7}\text{As}$ and $x = 0.516 \pm 0.05$ and $R = 97\%$ for $\text{In}_{0.52}\text{Ga}_{0.48}\text{As}$, respectively.

4 Conclusion

We found that surface morphology, crystal quality, and composition of InGaP sensitively depended on growth temperature, V/III, and III_(In)/III_(Ga) ratios due to high thermal decomposition temperature of PH_3 source and due to the difference in bonding energy between In-P and Ga-P bonds. It is found that the bandgap of InGaP can be tuned not only by In composition but also by ordering parameter, which is dependent on growth conditions. However, the high crystal quality and smooth

surface $\text{In}_{0.5}\text{Ga}_{0.5}\text{P}$ for 1.9-eV top cell has been obtained by controlling growth conditions carefully. Besides, the effects of misfit gradient in metamorphic SG buffer layer have been investigated for the growth of 1- and 0.75-eV InGaAs-based subcells. By designing multiple discrete strained layers in metamorphic buffer structure, TDs were blocked effectively through annihilation reactions between TDs or TD blocked by MD mechanisms as predicted in theoretical models. The use of higher misfit gradient to design $\text{In}_x\text{Ga}_{1-x}\text{As}$ metamorphic buffer results in less effective TD blocking, though the buffer layer thickness was reduced to about 600 nm. The buffer layer structure including 8-SG InGaAs with nonlinear indium gradient was found to be the optimal for blocking TDs more efficiently for growing 1-eV InGaAs on 1.4-eV GaAs middle cell, while the buffer layer thickness was maintained to be lower than 1 μm . The use of similar buffer structure to subsequently grow 0.75-eV InGaAs subcell was also impressive in positive achievements. TEM images confirmed that TDs as low as $1 \times 10^6 \text{ cm}^{-2}$ on 1- and 0.75-eV InGaAs active layers have been observed. We are going to combine results from this work and results from previous work to fabricate full 4-junction IMM solar cell structure in the next step. We also believe that metamorphic growth technique developed from this study can be applied for future 5- or 6-junction IMM solar cell.

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