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Control of threading dislocations by strain engineering in GaInP buffers grown on GaAs substrates

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ABSTRACT

High quality strain-relaxed In0.3Ga0.7As layers with threading dislocation density about 2×10^6 cm^{-2} and root-mean-square surface roughness below 8.0 nm were obtained on GaAs substrates using compositionally undulating step-graded $Ga_{1-x}In_xP$ ($x = 0.48$–0.78) buffers. The transmission electron microscopy results reveal that the conventional step-graded GaInP buffers produce high density dislocation pile-ups, which are induced by the blocking effect of the nonuniform misfit dislocation strain field and crosshatched surface on the gliding of threading dislocations. In contrast, due to strain compensation, insertion of the tensile GaInP layers decreases the surface roughness and promotes dislocation annihilation in the interfaces, and eventually reduces the threading dislocation density. This provides a promising way to achieve a virtual substrate with the desired lattice parameter for metamorphic device applications.

1. Introduction

In group III–V material systems, band gap engineering has been constrained largely by the limited substrate lattice parameter, which prevents the growth of defect free heterostructures in the case of large lattice misfit. The metamorphic growth has attracted growing interest due to the formation of virtual substrates with the desired lattice constant to favor the designs of semiconductor devices. In the strain relaxation process of metamorphic growth, threading dislocations (TDs) are concomitantly generated with misfit dislocations (MDs). Acting as nonradiative recombination or scattering centers to reduce the carrier lifetime [1], TDs are detrimental to optoelectronic devices, e.g., solar cells, lasers, and light emitting diodes. Thus, it is crucial to prevent TDs from penetrating into the device active regions as much as possible by utilizing suitable metamorphic buffer layers. Various buffer structures have been implemented to reduce the TD density, including a thick uniform buffer [2], a compositionally linearly-graded, step-graded, or reverse-graded buffer [3–5], and a digitally graded buffer [6]. Besides those, overshoot [7] or reverse steps [8] on the top buffer, Be doping [9] or dilute nitride incorporation [10] into the buffer was also proved to be beneficial for the strain relaxation and TD reduction. The compositionally step-graded $Ga_xIn_{1-x}P$ ($x = 0.52$–0.22) buffer has been used in triple-junction $Ga_{0.52}In_{0.48}P/GaAs/In_{0.3}Ga_{0.7}As$ solar cells to bridge the 2.2% lattice mismatch between GaAs and $In_{0.3}Ga_{0.7}As$ epilayers [11]. Although the TD density has been significantly reduced by suppressing phase separation in the metamorphic GaInP buffer [12], the buffer structure needs to be further optimized to obtain high quality $In_{0.3}Ga_{0.7}As$ layers with lower TD density and smaller surface roughness. In this work, we insert some reverse step GaInP layers with tension strain in the common compressive step-graded GaInP buffer (increasing the In content by steps) to improve the quality of the InGaAs layer on top of it, and the results show that this buffer not only decreases the surface roughness but also reduces the TD density of the InGaAs cap layer to about 2×10^6 cm^{-2}. This compositionally undulating buffer structure provides a promising way for metamorphic buffer growths.

2. Experiments

The experimental samples under investigation were grown on Si-doped GaAs substrates with 15° miscut toward (111)A by low-pressure (10^4 Pa) metal–organic chemical vapor deposition (MOCVD) using trimethylindium and trimethylgallium as the group-III precursors, PH_3 and AsH_3 as the group-V sources, and palladium diffused H_2 as the carrier gas. The schematic diagrams of the conventional step-graded (SG) and undulating step-graded (USG) buffer structures are shown in Fig. 1. Initially, a 100 nm thick GaAs layer was deposited to smooth the surface. Then, the metamorphic buffer layers were grown at 610 °C, subsequently a 1.0 μm thick InGaAs cap layer lattice-matched to the top buffer layer was grown at 675 °C. No interruption was employed in the buffer growth and during the temperature ramp from 610 °C to 675 °C. The average growth rate of the buffer was

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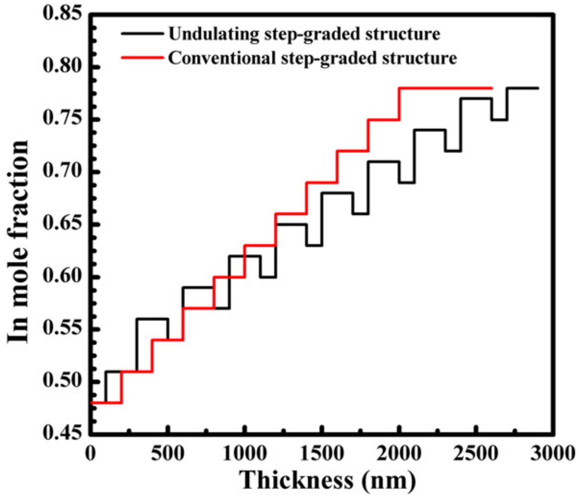

Fig. 1. Schematic diagrams of the SG and USG buffer structures. In the SG buffer, the In mole fraction was increased monotonically by steps. In the USG buffer, tensile GaInP layers were inserted between the compressive GaInP layers.

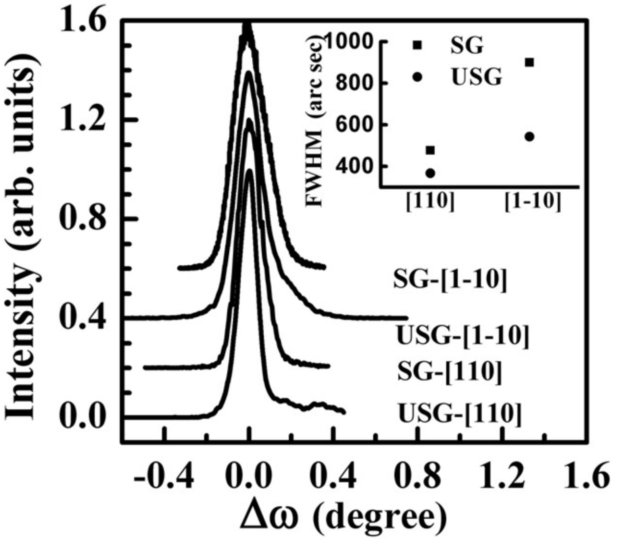

Fig. 2. (004) rocking curves of InGaAs cap layers of the SG and USG samples with the incident X-ray beam along the [110] and [1-10] directions. The inset shows the FWHM of each rocking curve.

about 0.55 nm/s and the V/III ratio was kept at 108 by simultaneously adjusting the In- and PH_3-fluxes.

The degree of the strain relaxation and crystalline quality of the InGaAs layers were characterized by X-ray diffraction using a Bruker D8 high resolution X-ray diffractometer with a 2 kW sealed X-ray tube and the wavelength is about 0.154 nm (Cu Kα1). The sample was mounted on a four-axis sample holder, in which each axis was controlled by a stepper motor. The surface texture and root-mean-square (RMS) roughness were examined using a Veeco Dimension 3100 atomic force microscopy (AFM) system with the Nanoscope IIId controller in tapping mode. The crystal microstructures and dislocation distributions were evaluated by transmission electron microscopy (TEM) in cross section (XTEM) and plan view (PVTEM) using a Tecnai G2 F20 S-Twin microscope operated at 200 kV. XTEM samples were cleaved along <110> directions. All the XTEM and PVTEM samples were manually polished to about 10 μm and further thinned by ion milling (Ar-ion guns). The photoluminescence (PL) measurements were performed by an RPM 2000 mapping system with a 980 nm excitation laser.

3. Results and discussions

Fig. 2 shows the (004) rocking curves of the InGaAs cap layers growing on the SG and USG GaInP buffers with the incident X-ray beam along the [110] and [1-10] directions. In compressively strained zinc blende semiconductors with lattice mismatch less than 1.5%, the misfit strain is mainly relieved by α and β dislocations (which belong to 60° dislocations) with group III and V atoms at their core and line vector along the [1-10] and [110] directions [13], respectively. The broadening of the (004) rocking curves is mainly attributed to the dislocations with line vector normal to the incident X-ray beam, i.e., the full width at half maximum (FWHM) of the rocking curves measured at the [110] azimuth reflects the α dislocation density while that in the perpendicular direction corresponds to the β dislocation density [14]. As shown in the inset of Fig. 2, the FWHM of the USG sample (sample using the USG buffer) measured along the [110] direction decreases from 474 arc sec to 364 arc sec and from 900 arc sec to 544 arc sec along the [1-10] direction in comparison with the SG sample (sample using the SG buffer), demonstrating that the α and β dislocation densities are reduced by 41% and 63%, respectively, since the dislocation density is proportional to the square of the corresponding FWHM [15]. Given in Fig. 3 are the PL spectra of the InGaAs cap layers. Although both samples have the desired energy bandgap ~1.03 eV, the PL peak intensity of the SG sample is roughly half that of the USG sample, meaning much more TDs in the SG sample as nonradiative recombination centers. This is consistent with the rocking curve results shown in Fig. 2. In metamorphic buffers, the lattice mismatch *f* equals to the sum of the elastic strain ε (the residual strain) and the plastic strain δ (the relieved strain). As shown in Table 1, the plastic strain δ of the SG and USG samples obtained from the symmetric (004) and asymmetric (224) reciprocal space mappings (RSMs) is almost identical. Thus, the lower TD density in the USG sample is closely associated with the buffer structure rather than the difference in the relieved strain in comparison with the SG sample.

The PVTEM micrograph with the diffraction vector **g** = <220> in Fig. 4(a) exhibits that the dislocations in the SG sample distribute nonuniformly in the form of pile-ups and the TD pile-up density is over 2×10^7 cm^{-2} on average over 5×5 μm^2. However, as shown in Fig. 4(b), the TDs in the USG sample distribute uniformly and the TD density is below 2×10^6 cm^{-2} estimated over 10×10 μm^2. Thus, the higher TD density in the SG sample is mainly attributed to the generation of dislocation pile-ups. In metamorphic buffers, dislocation pile-ups mainly derive from a combination effect of dislocation–dislocation interactions and the adverse effect of surface morphology roughening on dislocation glide [16]. Fig. 5 shows the PVTEM micrograph of the SG sample with the diffraction vector **g** = <1-31>. It can be seen that some pile-ups locate around the cross points between the lines along

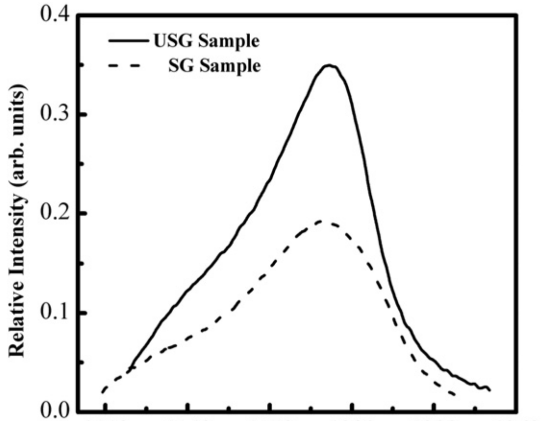

Fig. 3. PL spectra of the InGaAs cap layers of the SG sample (dashed line) and the USG sample (solid line) measured at room temperature.