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Threading Dislocation Blocking in Metamorphic InGaAs/GaAs for Growing High-Quality $In_{0.5}Ga_{0.5}As$ and $In_{0.3}Ga_{0.7}As$ on GaAs Substrate by Using Metal Organic Chemical Vapor Deposition

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High quality $In_{0.3}Ga_{0.7}As$ and $In_{0.51}Ga_{0.49}As$ epilayers have been successfully grown on the GaAs substrate by MOCVD. A cross-sectional study by transmission electron microscopy showed that the threading dislocations (TDs) have been successfully contained and limited within the buffer layers designed to stop the elongation of TDs into the $In_{0.3}Ga_{0.7}As$ and $In_{0.51}Ga_{0.49}As$ epilayers. A TD density of $1 \times 10^6\,cm^{-2}$ in a fully relaxed $In_{0.51}Ga_{0.49}As$ epilayer was achieved. The measurement of lifetimes of n- and p-type $In_{0.51}Ga_{0.49}As$ has been done by using time-resolved photoluminescence. A great reduction in the number of recombination centers in the InGaAs epilayer has been shown.

The ternary compounds of $In_xGa_{1-x}As$ on GaAs substrate have attracted considerable interest for a wide variety of electronic and photovoltaic device applications.[1)] Particularly for III–V-based photovoltaic devices, 1.05 and 0.75 eV $In_xGa_{1-x}As$ compounds play an important role in device structures.[2)] However, the high lattice mismatch between $In_xGa_{1-x}As$ compounds and GaAs substrate obstructs the growth of a high-quality epilayer, especially using metal organic chemical vapor deposition (MOCVD). In the growth of lattice-mismatched epitaxial films, threading dislocations (TDs) are concomitantly generated with misfit dislocations (MDs).[3)] For minority carrier devices, TDs are deleterious to the performance of devices because they provide a large number of traps at which electrical carriers can recombine.[3,4)]

To date, there has been a great amount of publications that discussed the theories of the formation, gliding, and blocking of TDs in metamorphic structures.[5–7)] It is believed that the TD density can be reduced through reaction with other TDs.[8)] Romanov *et al.*[9)] theoretically suggested that the use of multiple discrete strained layers can result in a marked reduction in TD density through annihilation reactions between TDs.[9)] According to their report, once the discrete strained layers were grown exceeding their critical thickness, TDs generated with MDs may fall within an annihilation radius,[9)] at which point TDs annihilate. In particular, InGaAs/GaAs heterostructure has been strongly investigated for the reduction of TD density in graded composition InGaAs/GaAs by molecular beam epitaxial (MBE) growth.[10–14)] It has been shown that the most effective way to reduce the TDs density in epilayers is to optimize the design of the concentration profile of linear and nonlinear continuously graded buffer layers in order to reduce TDs. However, not much attention has been paid to the step-graded buffers with a parabola-like composition profile for over 50% indium composition in InGaAs compound on GaAs substrates by MOCVD.

In this paper, we investigate the TD blocking method in the InGaAs/GaAs system for growing high-quality $In_{0.3}Ga_{0.7}As$ and $In_{0.51}Ga_{0.49}As$ films by designing step-graded buffers with a parabola-like composition profile for $In_xGa_{1-x}As$ buffer layers. The buffer layers include eight layers of $In_xGa_{1-x}As$. The indium composition was increased rapidly starting from $x = 0.05$–0.29 at the final step of buffer growth before a 2 μm $In_{0.3}Ga_{0.7}As$ epifilm was grown on the top. Two sets of buffer layers have been deposited on separate samples. The thickness of an individual layer in the buffer layer for set one is adjusted to a value below its critical thickness; meanwhile, the second one was set to exceed the critical thickness. The critical thickness of an individual layer was estimated based on the Matthews–Blakeslee (MB) model[15)] using eq. (1).

$$h_c = \frac{|b|}{8\pi\varepsilon_m \cos\lambda}\left(\frac{1-\nu\cos^2\beta}{1+\nu}\right)\ln\left(\frac{\alpha h_c}{|b|}\right). \qquad (1)$$

Equation (1) can be simplified to $h_c = |b|/\varepsilon_m$ because the product of all the other terms in eq. (1) is approximately constant and have magnitude on the order of one,[9)] where $|b|$ is the magnitude of the Burger vector b, ε_m is the misfit strain, λ is the angle between the Burgers vector and the line in the interface plane that is perpendicular to the intersection of the glide plane with the interface, β is the angle between the Burgers vector and the line vector for the dislocations, ν is the Poisson ratio and α is the core cutoff parameter.

This experiment was carried out by using epiready GaAs(001) substrates with 6° off-cut[16)] toward the [110] direction. Metal organic chemical vapor deposition (MOCVD-EMCORE D180) was used to grow the epilayers. Group-III precursors of trimethylindium (TMIn) and trimethylgallium (TMGa) and the group-V precursor of pure arsine (AsH_3) were used. Monosilane (SiH_4) and carbon tetrabromide (CBr_4) were used as n- and p-type doping sources. The total pressure in the reactor and growth temperature were kept at 70 Torr and 490 °C, respectively. 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 two-beam condition cross-sectional and plan-view transmission electron microscopy (TEM). Minority carrier lifetimes were examined by time-resolved photoluminescence (TR-PL) with a titanium-sapphire laser excitation source.

Figures 1(a) and 1(b) show the cross-sectional two-beam bright field TEM images taken near the [011] zone axis with

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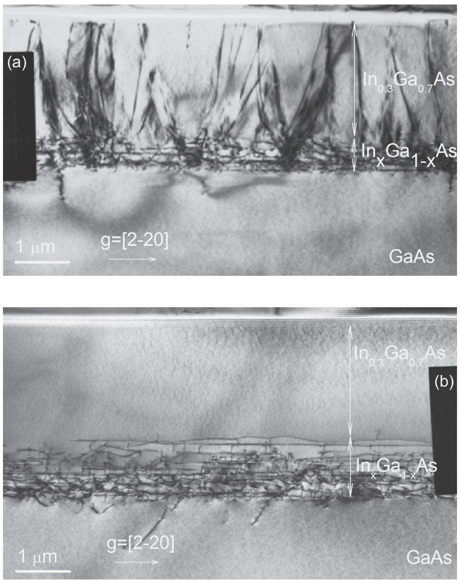

Fig. 1. Cross-sectional two-beam bright-field TEM images of $In_{0.3}Ga_{0.7}As$ film grown on 6° off-cut toward [110] GaAs substrate using (a) 600 nm and (b) 1.3 µm $In_xGa_{1-x}As$ buffer layers.

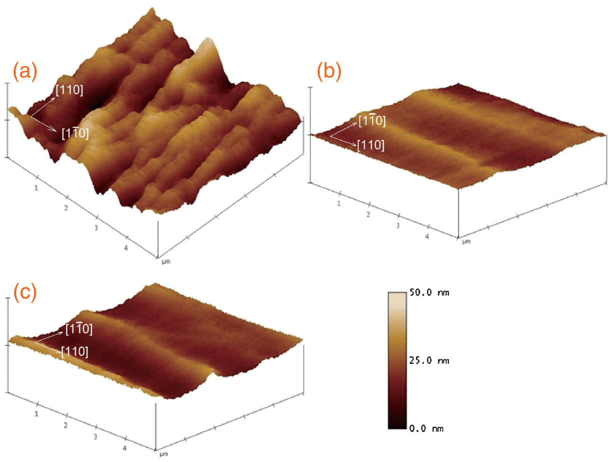

Fig. 2. AFM images of $In_{0.3}Ga_{0.7}As$ films grown on 6° misorientation toward [110] GaAs substrate using (a) 600 nm and (b) 1.3 µm $In_xGa_{1-x}As$ buffer layers, and (c) is the AFM image of $In_{0.51}Ga_{0.49}As$ film.

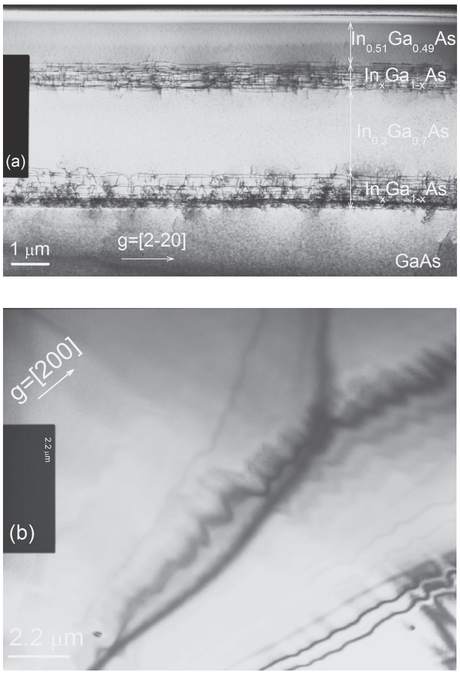

Fig. 3. (a) Cross-sectional two-beam bright-field TEM image of $In_{0.51}Ga_{0.49}As$ film grown on 6° off-cut toward [110] GaAs substrate, (b) plan-view bright-field TEM image of the sample.

$g = [2\bar{2}0]$ of $In_{0.3}Ga_{0.7}As$ samples grown on GaAs substrate using the eight-step graded strained buffer $In_xGa_{1-x}As$ layers. It is clearly shown in Fig. 1(a) that TDs could not be confined within the buffer layer when the thickness of each step buffer layer was set to about 65 nm. They elongated or propagated to the top free surface. The high TD density extended from the bottom layers has worsened the surface morphology of the top surface layer. An AFM study [Fig. 2(a)] has shown the surface morphology with the root mean square (RMS) roughness of 8.3 nm. In contrast, as shown in Fig. 1(b), no obvious TD was observed in the $In_{0.3}Ga_{0.7}As$ on top of the graded buffer layers when the thickness of the individual layer within the graded buffer layers was about 150 nm. It is clear that TDs were blocked and contained within the graded buffer layers, resulting in almost no TD extention into the epilayer on top. In addition, the high-quality $In_{0.3}Ga_{0.7}As$ epilayers also improved the surface morphology. As shown in Fig. 2(b), a mirrorlike surface with RSM roughness of 1.5 nm has been obtained. The lower TD density in the epilayer resulted from the annihilation reactions between TDs,[9] which can be seen when observing the buffer layer in detail. The results observed are experimental evidence in support of the mechanism of annihilation reaction between TDs, which was described in detail in refs. 8 and 9. Simultaneously, TDs blocked by MDs were observed, especially in the upper buffer layers. In addition, a large clean region was formed with long MDs that increased the possibility of TD annihilation.[12] The results obtained are clear evidence in support of Freund's blocking model.[6]

Understanding the mechanism and process of TD blocking by $In_xGa_{1-x}As$ buffer layers allows us to optimize the buffer design to achieve a high-quality $In_{0.51}Ga_{0.49}As$ epilayer. Figure 3(a) shows a cross-sectional bright-field TEM image of 1.3 µm n-type-doped $In_{0.51}Ga_{0.49}As$ grown continuously on $In_{0.3}Ga_{0.7}As$ using six $In_xGa_{1-x}As$ ($x = 0.34$–0.50) layers. The thickness of each layer in the buffer layers is about 150 nm. No TDs were observed on the $In_{0.51}Ga_{0.49}As$ epilayer in the range of 12 µm. This suggests that the TD density in the top layer could be lower than 1×10^3 cm^{-1}. The plan-view TEM image in Fig. 3(b), taken with $g = [200]$ near the [001] zone axis, shows only two threading dislocations on a large area of 200 µm^2, which indicates that a TD density of 1×10^6 cm^{-2} in $In_{0.51}Ga_{0.49}As$ was achieved. The growth of high indium composition $In_{0.51}Ga_{0.49}As$ also caused increased RSM roughness of the film to 3.3 nm [Fig. 2(c)].

Figure 4 represents the reciprocal space map (RSM) of the structure shown in Fig. 3(a). The diffracted intensity is measured around the asymmetric (115) reciprocal lattice point of the GaAs substrate. The reciprocal space separation

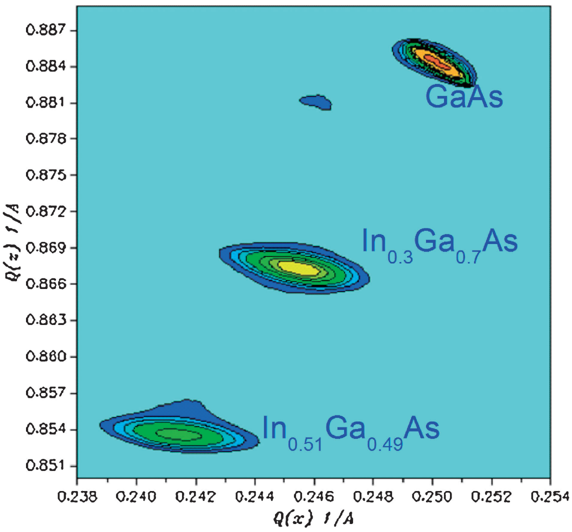

Fig. 4. Reciprocal space map (RSM) of $In_{0.51}Ga_{0.49}As/In_{0.3}Ga_{0.7}As$ measured around the asymmetric (115) reciprocal lattice point of GaAs substrate.

between the GaAs substrate and the two epilayers, which can be converted to real space, confirm the indium compositions in each epilayer. The RSM figure shows that $In_{0.3}Ga_{0.7}As$ and $In_{0.51}Ga_{0.49}As$ were almost fully relaxed on the GaAs substrate.

Finally, the minority carrier lifetime in the $In_{0.51}Ga_{0.49}As$ epilayer was examined by TR-PL measurement. A mode-locked titanium-sapphire (Ti:S) laser (XL200) tuned to 800-nm-wavelength output was used for this purpose, and the output luminescence signal was detected near the band gap of the material. The photoluminescence lifetime[17] is expressed in eq. (2),

$$1/\tau_{PL} = 1/\tau_r + 1/\tau_{nr} + 1/\tau_s, \qquad (2)$$

where $1/\tau_s = (S_1 + S_2)/d$, and τ_{PL} is the photoluminescence lifetime, τ_r is the radiative lifetime, τ_{nr} is the nonradiative lifetime, S_1 and S_2 are the interface recombination velocities, and d is the thickness of the active layer. Figure 5 illustrates the time-resolved photoluminescence of n- and p-type-doped $In_{0.51}Ga_{0.49}As$ with the doping concentration for both types being about $5 \times 10^{17}\,cm^{-3}$ determined by electrochemical capacitance–voltage (ECV) measurement. Carrier lifetimes were extrapolated by exponential decay fitting. The steep initial slopes with 90 and 110 ps decay times corresponding to n- and p-type dopings, respectively, were related to the high surface recombination velocities of the $In_{0.51}Ga_{0.49}As$ free surface and interface between $In_{0.51}Ga_{0.49}As$ and InGaAs buffer layers. 2.05 and 1.85 ns lifetimes of n- and p-type dopings, respectively, were expected to be related to radiative lifetimes, which confirms that a low trap density in the epifilm has been achieved.

In a summary, threading dislocations have been successfully confined and blocked within designed graded strained $In_xGa_{1-x}As$ buffer layers with parabolic increment in indium composition. No propagation of TDs was seen in the subsequently grown $In_{0.3}Ga_{0.7}As$ and $In_{0.51}Ga_{0.49}As$ epilayers. The use of a thickness exceeding the critical thickness for an individual layer in graded buffer layer sets has induced the annihilation reaction among TDs and the blocking of TDs by MDs. The result was that TD densities as low as $1 \times 10^6\,cm^{-2}$ in $In_{0.51}Ga_{0.49}As$ has been achieved. Epilayers with better crystal quality have greatly improved their surface morphology. Almost perfectly flat mirrorlike surfaces were obtained on $In_{0.3}Ga_{0.7}As$ and $In_{0.51}Ga_{0.49}As$ with RMS roughnesses of 1.5 and 3.3 nm, respectively. TR-PL measurement has determined radiative lifetimes of about 2 ns for both n- and p-type-doped $In_{0.51}Ga_{0.49}As$ epilayers, indirectly indicating that the epilayers have very low radiative recombination centers.

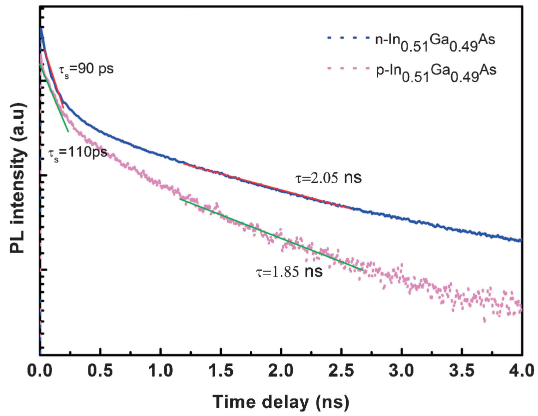

Fig. 5. Room temperature time-resolved photoluminescence measurements for n- and p-type-doped $In_{0.51}Ga_{0.49}As$ films. The solid lines show the exponential fit for both decays.

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