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Strain relaxation of the In$_{0.53}$Ga$_{0.47}$As epi-layer grown on Si substrate by molecular beam epitaxy

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Abstract: The In$_{0.53}$Ga$_{0.47}$As films were grown on the Si (111) substrate with two different In$_x$Ga$_{1-x}$As buffer layers by molecular beam epitaxy (MBE). The effect of buffer layer on the as-grown In$_{0.53}$Ga$_{0.47}$As epi-layers was investigated by X-ray diffraction (XRD), reciprocal space mapping (RSM), Raman and transmission electron microscopy (TEM). XRD results showed that the crystalline quality of as-grown In$_{0.53}$Ga$_{0.47}$As epi-layer grown on Si substrate by using low-temperature In$_{0.4}$Ga$_{0.6}$As buffer layer with in-situ annealing was better than that by using In$_{0.2}$Ga$_{0.8}$As/In$_{0.4}$Ga$_{0.6}$As buffer layers. Moreover, the misfit strain between In$_{0.53}$Ga$_{0.47}$As epi-layers and Si substrate was nearly completely released by inserting a single In$_{0.4}$Ga$_{0.6}$As buffer layer grown at 390 °C with in-situ annealing at 560 °C. Specifically, the relaxation value of the In$_{0.53}$Ga$_{0.47}$As epi-layer with the single In$_{0.4}$Ga$_{0.6}$As buffer layer was 97.16 %. The lattice mismatch strain of the In$_{0.53}$Ga$_{0.47}$As epi-layer was well confined to the In$_{0.4}$Ga$_{0.6}$As buffer layer, without extended to the subsequently grown In$_{0.53}$Ga$_{0.47}$As epi-layer compared with its counterpart using the In$_{0.2}$Ga$_{0.8}$As/In$_{0.4}$Ga$_{0.6}$As buffer layers. The low-temperature In$_{0.4}$Ga$_{0.6}$As buffer layer shows a way to realize high crystalline quality and fully relaxed In$_{0.53}$Ga$_{0.47}$As films on the Si substrate.

Key words: In$_{0.53}$Ga$_{0.47}$As, stress relaxation, dislocation, molecular beam epitaxy

1. Introductions

The heteroepitaxy of In$_x$Ga$_{1-x}$As films on various types of substrates is widely used in many advanced electronic and optoelectronic applications, mainly for the following two reasons. Firstly, the energy band gap ($E_g$) of In$_x$Ga$_{1-x}$As material covers the range from 0.36 (InAs) to 1.42 eV (GaAs) which is suitable for high-efficiency solar cells,$^1$ laser diodes,$^2$ photodetectors,$^3-5$ and so on. Moreover, the In$_x$Ga$_{1-x}$As material has high carrier mobility which is essential for high-speed electronic devices.$^6,7$ In particular, In$_{0.53}$Ga$_{0.47}$As is an ideal III-V compound semiconductor for a metal-oxide-semiconductor field-effect transistor (MOSFET) channel material due
to its high electronic mobility and high breakdown field. However, the performance of the device is mainly influenced by the crystalline quality of In$_{0.53}$Ga$_{0.47}$As. Therefore, improving the crystalline quality is a key issue for high-performance III-V MOSFET. In general, the InP and GaAs are most commonly used as substrates for the growth of In$_{0.53}$Ga$_{0.47}$As due to the lattice matching between them. Unfortunately, the InP and GaAs substrates have their disadvantages such as high cost, small size and large brittleness. Undoubtedly, the Si wafers are most widely utilized as the substrates in the micro-electronics and large scale integrated circuits, and about 95% of all semiconductor devices are presently fabricated using Si. A Si wafer as the carrier, is considerably advantageous due to its higher thermal conductivity, low cost, large size and very mature process technology. Therefore, the researchers considered using Si as an alternative for the epitaxy of In$_{0.53}$Ga$_{0.47}$As film. However, the intrinsic strain typically arises due to the constraint of heteroepitaxy considering the different lattice parameters between the epi-film and the substrate. If In$_{0.53}$Ga$_{0.47}$As is directly grown on Si, a great number of defects will be generated in the as-grown In$_{0.53}$Ga$_{0.47}$As film due to the large lattice mismatch, ultimately leading to a deteriorated device performance. In order to obtain better relaxation and high-quality In$_{0.53}$Ga$_{0.47}$As epitaxial films on the Si substrate, one effective way is to use buffer layers to reduce the stress caused by lattice mismatch between them. Therefore, the structure and epitaxial growth procedures of buffer layers are of paramount importance to achieve high-quality In$_{0.53}$Ga$_{0.47}$As films on Si.

In this work, we report on the growth of In$_{0.53}$Ga$_{0.47}$As epitaxial films on 2-inch Si (111) substrate by molecular beam epitaxy (MBE) using composition-graded In$_{0.2}$Ga$_{0.8}$As/In$_{0.4}$Ga$_{0.6}$As buffer layers and a single In$_{0.4}$Ga$_{0.6}$As buffer layer, respectively. Two samples using these two different buffer layers were grown to compare the strain relaxation. The investigation results showed that the buffer layers have great effect on the strain relaxation during the heteroepitaxy. The better relaxation In$_{0.53}$Ga$_{0.47}$As epi-layer is the one grown on the In$_{0.4}$Ga$_{0.6}$As single buffer layer with a low growth temperature and in-situ annealing. This achievement is of great interest for a simple approach to achieve high-quality In$_{0.53}$Ga$_{0.47}$As films on the Si substrates.

2. Experimental details

The In$_{0.53}$Ga$_{0.47}$As films were grown on 2-inch diameter Si (111) substrates by MBE. High purity In (7N), Ga (7N) and As (7N) were used as the sources, respectively. The Si substrates were primarily ultrasonically cleaned with chemicals and deionized water to remove the surface contaminations and finally dried by 7N nitrogen gas before being put into the MBE load-lock chamber with a pressure of 3.2×10$^{-7}$ Torr. The substrates were then transferred into the high-vacuum MBE growth chamber under a pressure of 4.0×10$^{-10}$ Torr and annealed at 1000 °C for 30 min to remove the surface oxidized layer. Two samples were grown using buffer layers of different structures. For sample A, the composition-graded In$_{0.2}$Ga$_{0.8}$As/In$_{0.4}$Ga$_{0.6}$As buffer layers were utilized for the epitaxy of In$_{0.53}$Ga$_{0.47}$As. Each sub-layer thickness of buffer layer was ~ 6 nm and the growth temperature was remained at 560 °C.
composition-graded In$_{0.2}$Ga$_{0.8}$As/In$_{0.4}$Ga$_{0.6}$As buffer layers of 12 nm were grown in total thickness. In order to study the effect of the buffer layer on the In$_{0.53}$Ga$_{0.47}$As film crystalline quality, the buffer layer was grown at a low temperature for comparison. For sample B, a single In$_{0.4}$Ga$_{0.6}$As buffer layer of 12 nm was grown before the subsequent epitaxy of the In$_{0.53}$Ga$_{0.47}$As film. The growth temperature of buffer layer was 390 °C with a 5 min in-situ post-annealing at 560 °C. The substrate temperature was then fixed to 560 °C and a 100 nm thick In$_{0.53}$Ga$_{0.47}$As layer was grown afterwards for both samples. The crystallinity of as-grown films were characterized by high-resolution X-ray diffraction (XRD) with Cu Kα$_1$ as the X-ray source (Bruker D8 Discover). Raman spectra was obtained at room temperature using 514.5-nm line of Ar$^+$ laser as an exciting source. Transmission electron microscopy (TEM, JEOL 3000F) was carried out to study the microstructure of the samples. The field emission gun of TEM was working at a voltage of 300 kV, which gave a point to point resolution of 0.17 nm.

3. Results and discussions

The structural properties of as-grown In$_{0.53}$Ga$_{0.47}$As films on Si (111) substrate were investigated by XRD. Fig. 1(a) shows the typical XRD patterns of sample A. We have confirmed the In$_{0.53}$Ga$_{0.47}$As epi-layers from diffraction angle. Except for the diffraction peaks from In$_{0.53}$Ga$_{0.47}$As (111) and the Si (111) substrate, no other diffraction peaks are detected, which confirms that the In$_{0.53}$Ga$_{0.47}$As epi-layer is single crystalline. The influence of buffer layer on the crystalline quality of as-grown In$_{0.53}$Ga$_{0.47}$As epi-layers is studied by X-ray rocking curves (XRCs). Fig. 1(b) represents the XRCs for In$_{0.53}$Ga$_{0.47}$As epi-layers (111) grown on Si (111) substrates using two different buffer layers, from which the crystalline quality of as-grown In$_{0.53}$Ga$_{0.47}$As could be evaluated. The full-width at half-maximums (FWHMs) are about 595.56 and 556.41 arcsec for as-grown In$_{0.53}$Ga$_{0.47}$As epi-layers with the sample A and B, respectively. Apparently, In$_{0.53}$Ga$_{0.47}$As grown on Si (111) with the low-temperature and in-situ annealing In$_{0.4}$Ga$_{0.6}$As buffer layer exhibits higher crystallinity than that grown with composition-graded buffer layers.

![Fig. 1(a)](image1.png) Typical XRD analysis of sample A using composition-graded buffer layers, (b) XRCs of as-grown In$_{0.53}$Ga$_{0.47}$As (111) planes for sample A and B, respectively.
In order to study the strain state of the epitaxial In$_{0.53}$Ga$_{0.47}$As films, reciprocal space mappings (RSMs) measurement was carried out for both the symmetric (111) and asymmetric (224) planes of the 100 nm thick In$_{0.53}$Ga$_{0.47}$As films, as shown in Fig. 2. The reciprocal space coordinates in this paper are denoted as ($q_x$, $q_z$) which are transformed from the real space angles.

![Fig. 2 The RSMs of In$_{0.53}$Ga$_{0.47}$As films grown on Si using two different buffer layers for sample A (a, b) and sample B (c, d), respectively.](image)

Fig. 2(a)-(b) present RSMs results of sample A for the diffraction plane of (111) and (224), respectively. It is distinctly observed from Fig. 2(a) that the In$_{0.53}$Ga$_{0.47}$As (111) layer are sitting rightly behind Si (111) substrate in the reciprocal space, indicating the epitaxial relationship of In$_{0.53}$Ga$_{0.47}$As (111) || Si (111). Besides, the diffraction patterns of the Si (111) substrate and the In$_{0.53}$Ga$_{0.47}$As epitaxial layer are well resolved. The In$_{0.53}$Ga$_{0.47}$As film displays an elliptically shaped diffraction pattern, which can be attributed to the mosaic structure of the epi-layer, crystallographic tilt of the epi-layer, and the crystalline distortion. Fig. 2(b) shows the asymmetric (224) RSM of the samples A with the composition-graded buffers. We can clearly observe that the diffraction peaks of In$_{0.53}$Ga$_{0.47}$As (224) presents an obvious broadening along the mosaic direction. The (111) RSM of sample B in Fig. 2(c) also reveals the epitaxial relationship of In$_{0.53}$Ga$_{0.47}$As (111) || Si (111). However, the (111) RSM diffraction pattern of the In$_{0.53}$Ga$_{0.47}$As film displays an approximately circle shape, which manifests an improved crystalline quality of the In$_{0.53}$Ga$_{0.47}$As films using a single In$_{0.4}$Ga$_{0.6}$As buffer layer. The asymmetric (224) RSM of the sample B are shown in Fig. 2(d), which also exhibits a broaden elliptical shape along
the mosaic direction. It has been reported that broadening of the peak in various directions is due to the crystal imperfections. Diffraction peak broadening along the mosaic direction was an indication of the presence of mosaic blocks which slightly rotate the allowable diffraction plane in their vicinity.\(^\text{15}\)

In order to further verify the relaxation state of the as-grown In\(_{0.53}\)Ga\(_{0.47}\)As films, we have calculated the relaxation value of the In\(_{0.53}\)Ga\(_{0.47}\)As epi-layers. As we know, the lattice constant of In\(_{x}\)Ga\(_{1-x}\)As (0<x<1, 5.6533<a<6.0584 Å) material is larger than that of Si (a = 5.4310 Å) which results in compressively strained as-grown In\(_{0.53}\)Ga\(_{0.47}\)As film. The relaxed lattice constants of the epitaxial layer are then calculated by assuming a linear interpolation (Vegard’s law) between the lattice constants of the binary alloy constituents (GaAs and InAs).\(^\text{16}\) The lattice constant and the misfit strain to Si substrate for In\(_{x}\)Ga\(_{1-x}\)As employed in this work as shown in Table 1.\(^\text{17}\) Therefore, the lattice parameter of the fully relaxed In\(_{0.53}\)Ga\(_{0.47}\)As epi-layer can be calculated to be \(a_0^l = 5.8680\) Å. On the other hand, the lattice parameter of the In\(_{0.53}\)Ga\(_{0.47}\)As epi-layers can be derived according to the RSM results.\(^\text{18}\) Therefore, the lattice parameter of as-grown In\(_{0.53}\)Ga\(_{0.47}\)As films for samples A and B are \(a_1^l = 5.8206±0.0047\) and 5.8470±0.0086 Å, respectively. Additionally, the layer relaxation value \(R\), can be defined by:\(^\text{14}\)

\[
R = \frac{a_0^l - a_s^l}{a_0^l - a_s^0}
\]  

where \(a_1^l\) is the strained layer lattice parameter, and \(a_0^l\) and \(a_0^s\) are the fully relaxed lattice parameters of substrate and epi-layer, respectively. Thus, the relaxation values of the In\(_{0.53}\)Ga\(_{0.47}\)As epi-layers for sample A and B are \(R = 89.15±1.08\) % and 95.19±1.97 %, respectively. This result indicated that the better relaxation In\(_{0.53}\)Ga\(_{0.47}\)As epi-layer was grown on the In\(_{0.4}\)Ga\(_{0.6}\)As single buffer layer with a low growth temperature and in-situ annealing, compared to the sample A with the composition-graded buffer layers.

Table 1 Lattice constant and the misfit strain between the Si and In\(_x\)Ga\(_{1-x}\)As employed materials in this work.

<table>
<thead>
<tr>
<th>Material</th>
<th>Lattice constant (Å)</th>
<th>Misfit (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Si</td>
<td>5.4310</td>
<td>0</td>
</tr>
<tr>
<td>GaAs</td>
<td>5.6533</td>
<td>4.09</td>
</tr>
<tr>
<td>InAs</td>
<td>6.0584</td>
<td>11.55</td>
</tr>
<tr>
<td>In(<em>{0.2})Ga(</em>{0.8})As</td>
<td>5.7343</td>
<td>5.58</td>
</tr>
<tr>
<td>In(<em>{0.4})Ga(</em>{0.6})As</td>
<td>5.8153</td>
<td>7.08</td>
</tr>
<tr>
<td>In(<em>{0.53})Ga(</em>{0.47})As</td>
<td>5.8680</td>
<td>8.05</td>
</tr>
</tbody>
</table>

Fig. 3 shows Raman spectra from the samples with two different buffer layers. The first order Raman spectrum of a semiconductor typically reveal the longitudinal optical (LO) and transversal optical (TO) phonons information.\(^\text{19}\) However, the
ternary compound semiconductor In\textsubscript{x}Ga\textsubscript{1-x}As shows two-mode behavior in the first order Raman scattering, which are LO and TO phonons corresponding to both InAs and GaAs binary parent materials, and the frequency positions depend on the In composition (x).\textsuperscript{20-22} Fig. 3 shows Raman spectra of the In\textsubscript{0.53}Ga\textsubscript{0.47}As epi-layers with different buffer layers. For both samples of A and B, two strong peaks located at 226 cm\textsuperscript{-1} and 267 cm\textsuperscript{-1} occur, corresponding to TO phonon modes of InAs and LO phonon modes of GaAs, respectively. However, in the Raman spectra we can not clearly observe the peaks of LO\textsubscript{InAs} and TO\textsubscript{GaAs}, which are around 244 cm\textsuperscript{-1} and 254 cm\textsuperscript{-1}, respectively. The LO\textsubscript{InAs} and TO\textsubscript{GaAs} modes are related to disorder-activated lattice vibrations which are supposed to exist in In\textsubscript{0.53}Ga\textsubscript{0.47}As materials.\textsuperscript{22} The Raman results indicate high-crystallinity of the In\textsubscript{0.53}Ga\textsubscript{0.47}As epitaxial films obviously.

![Raman spectra](image)

**Fig. 3** Raman spectra of sample A (a) and B (b), respectively.

The evaluations of the stress of the In\textsubscript{x}Ga\textsubscript{1-x}As epi-layers are made from a frequency shift of the GaAs-like LO phonon.\textsuperscript{23} The GaAs-like LO phonon frequency $\Omega\textsubscript{LO}$ is blue-shifted for compressive layers ($\varepsilon<0$), between the values of the relaxed and fully strained material. The shifts are proportional to the residual strain $\varepsilon$, and depend on the In composition and the growth orientation,\textsuperscript{24}

$$
\Delta \Omega\textsubscript{LO(111)} = \Omega\textsubscript{uns} [(\tilde{K}\textsubscript{11} + 2\tilde{K}\textsubscript{12})(2 - r') - 4\tilde{K}\textsubscript{11}(1 + r')]\varepsilon / 6
$$

where

$$
r_{11} = (2C\textsubscript{11} + 4C\textsubscript{12} - 4C\textsubscript{44})/(C\textsubscript{11} + 2C\textsubscript{12} + 4C\textsubscript{44})
$$

$r'$ is the inverse of the Poisson ratio, which is dependent on the orientation, $C_{ij}$ is the elastic constants, $\tilde{K}_{ij}$ are the phonon deformation potentials of the In\textsubscript{0.53}Ga\textsubscript{0.47}As layer. The $C_{ij}$ and $\tilde{K}_{ij}$ have been linearly interpolated from data\textsuperscript{25} for InAs and GaAs.

The phonon frequency of the unstrained material has been determined on completely relaxed samples, with the result $\Omega\textsubscript{uns}=292.2-35.72x-14.82x^2$ at 300 K.\textsuperscript{24}
Using the measured results $\Delta \Omega_{1,0}$ and Eq. (1)-(2), it can be obtained that the stress of the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epilayers in samples A and B is -481.56 MPa and -371.29 MPa, respectively. This means the residual stress in the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ layers is compressive stress. The stress in epilayers mainly caused by the lattice mismatch between the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epilayer and Si substrate is decreased by using the buffer layers. And the residual stress of the sample B is lower than the sample A. Therefore, crystalline quality of the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epilayers can be improved by using the low temperature buffer layer with in-situ annealing growth on the Si substrate.

Fig. 4 Cross-sectional TEM images for sample A grown on Si substrate. (a) a bright field cross-sectional TEM image at low magnification for the interface between the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epitaxial layer and Si under the two-beam diffraction condition of $g=\{02\overline{2}\}$, (b) its corresponding high-resolution cross-sectional TEM micrograph around the interface, the inset is SAED image of the interface between the buffer layer and Si substrate, in which the solid lines marked in blue and pink are corresponding to diffraction planes of Si and buffer layer, respectively, and (c) magnified view of the $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layers.

Cross-sectional TEM investigation was carried out to investigate the structure of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ films grown on Si (111) substrate. Fig. 4(a) is a bright filed cross-sectional TEM image of sample A under the two-beam diffraction condition of $g=\{02\overline{2}\}$, where misfit dislocation and threading dislocation can be observed from their sharp contrast against the matrix, and the interface between the $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layers and Si substrate can also be clearly observed, as illustrated by the white dash-dot line. The buffer layers contain a much higher density of dislocations, which are along the interface. It can also be easily found that a high density of misfit dislocations occur in the vicinity of the interface between buffer layer and $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epilayer. From the selective area electron diffraction (SAED) of the interface, we obtain the epitaxial relationship between the buffer layer and Si.
substrate, which is $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$ (111) $\parallel$ Si (111), as shown in the insert of Fig. 4(b). Fig. 4(b) shows that thickness of the $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}$/$\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layers is about 12 nm, as illustrated by two white dash-dot lines. Furthermore, the compressive stress derived from the lattice mismatch can result in stacking faults along the epitaxial direction, which ultimately extend to the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epilayer, as shown by dash-line segment A in Fig. 4(b). As the epi-layer thickness gradually increases, the stacking faults are greatly decreased and even annihilated toward the epitaxial layer. In addition, the stacking faults have also been observed parallel to the direction of the interface at the buffer layer, as shown in Fig. 4(c), which its magnified view of the dash-line segment B of Fig. 4(b). Circles in Fig. 4(c) show the defects inside the buffer layer, and the high density of the defects in the buffer is detrimental to the subsequent growth of the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epitaxial layer.

Due to lattice mismatch between $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ and Si, the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ lattice is subjected to large compression strain from the Si lattice, leading to substantial mismatch stress at the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$/buffer layer and buffer layer/Si interface during epitaxial growth. In order to release the mismatch stress, misfit dislocations are generated at the buffer layer/Si and $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$/buffer layer interfaces. As the film thickness gradually increases, these interfacial misfit dislocations propagate and stretch upwards, resulting in the formation of threading dislocations and stacking fault. However, with increasing thickness of the epitaxial $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ film, the compression strain inside the film is gradually reduced and the threading dislocations can also be annihilated, as illustrated in Fig. 4(b).

Fig. 5 Cross-sectional TEM images for sample B grown on Si substrate. (a) a bright field cross-sectional TEM image at low magnification under the two-beam diffraction condition of g=[02-2], (b) high-resolution cross-sectional TEM micrograph around the interface, the inset is SAED image of the interface between the $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layer and Si substrate, in which the solid lines marked in blue and pink are corresponding to diffraction planes of Si and $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$, respectively, (c-e) magnified view of the $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layer in region I, II and III, respectively, and (f) high-resolution cross-sectional TEM micrograph of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epilayer.
Fig. 5 shows cross-sectional TEM images of sample B in which a single layer of In$_{0.4}$Ga$_{0.6}$As buffer layer is adopted. From Fig. 5(a) we can notice that the interface between Si (111) substrate and epi-layer is very abrupt. Fig. 5(b) is the typical high-resolution cross-sectional TEM image of sample B, although a high density of screw and edge dislocations is found in the In$_{0.4}$Ga$_{0.6}$As buffer layer, as illustrated by the circles, no threading dislocation occurs in the buffer layer. In addition, the epitaxial relationship of In$_{0.4}$Ga$_{0.6}$As (111) || Si (111) is distinctly illustrated from SAED patterns, as shown in Fig. 5(b) inset. In order to study the defect distribution in the buffer layer in details, three typical regions are selected and marked as I, II, and III in various positions of the buffer layer, as shown in Fig. 5(b). The magnified corresponding images are shown in Fig. 5(c)-(e), respectively. For region I, due to the lattice misfit of 7.08 % between In$_{0.4}$Ga$_{0.6}$As and Si, high density of defects especially lattice distortion arose in the vicinity of In$_{0.4}$Ga$_{0.6}$As/Si interface. On the other hand, Fig. 5(d) and 5(e) display high levels of stacking faults and dislocations. One of the most significant phenomena we have to pay attention is that although many defects such as lattice distortions and stacking faults can be found inside the In$_{0.4}$Ga$_{0.6}$As buffer layer, the interface of In$_{0.4}$Ga$_{0.6}$As/In$_{0.53}$Ga$_{0.47}$As is very abrupt with lower threading dislocation density, resulting in the high-crystallinity In$_{0.53}$Ga$_{0.47}$As epitaxial film. We can note that the In$_{0.53}$Ga$_{0.47}$As epitaxial film is of a high degree of structural perfection, as shown in Fig. 5(f).

We have tried to understand how the single In$_{0.4}$Ga$_{0.6}$As buffer layer can efficiently release misfit strain and trap dislocations by using low temperature growth and in-situ annealing. It has been reported that low-temperature buffer layer will provide low energy sites for the nucleation of dislocations and point defects, which, on the one hand, effectively prevents the propagation of these defects into the subsequent epi-layer and, on the other hand, releases the misfit strain between the substrate and epi-layer. Moreover, the atoms will rearrange within the buffer layer by the in-situ annealing process, which helps to release the misfit strain caused by lattice mismatch between the substrate and the subsequent In$_{0.53}$Ga$_{0.47}$As epi-layer. In this paper, the low-temperature single In$_{0.4}$Ga$_{0.6}$As buffer layer with in-situ annealing in this work will trap threading dislocation. Furthermore, it will introduce high density of defects within the In$_{0.4}$Ga$_{0.6}$As buffer layer to reduce the lattice misfit strain. In other words, although a very high density of point defects and dislocations are generated within the In$_{0.4}$Ga$_{0.6}$As buffer layer, the defects are confined in the In$_{0.4}$Ga$_{0.6}$As buffer layer, without extending to the subsequently grown In$_{0.53}$Ga$_{0.47}$As epi-layer.

4. Conclusions

To conclude, we have studied the structural properties of In$_{0.53}$Ga$_{0.47}$As films grown on Si (111) substrates with the composition-graded In$_{0.2}$Ga$_{0.8}$As/In$_{0.4}$Ga$_{0.6}$As buffer layers (sample A) and a single In$_{0.4}$Ga$_{0.6}$As buffer layer (sample B), respectively. The FWHMs from XRCs are about 595.56 and 556.41 arcsec for the as-grown two In$_{0.53}$Ga$_{0.47}$As (111) epi-layers, respectively, indicating that the crystalline quality of as-grown In$_{0.53}$Ga$_{0.47}$As epi-layers grown on Si substrate by
using low-temperature $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layer with in-situ annealing is better than that by using composition-graded $\text{In}_{0.2}\text{Ga}_{0.8}\text{As}/\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layers. RSMs have been used to study the strain relaxation value of as-grown $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ films with two different buffer layers. The relaxation value of as-grown $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epi-layers for sample A and sample B are 90.23 \% and 97.16 \%, respectively. Furthermore, the residual stresses derived from Raman spectra are calculated to be -481.56 MPa and -371.29 MPa for sample A and B, respectively. These results illustrate that the mismatch strain inside the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ layer can be effectively released by a single $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layer compared with the composition-graded buffer layer.

From TEM characterisation, we can further understand the strain relaxation mechanism and dislocation distribution of the buffer layers and epi-layers grown on Si substrate. For sample A, misfit dislocations are generated at the interfaces. As the film thickness gradually increases, these interfacial misfit dislocations propagate and stretch upwards, resulting in the formation of threading dislocations and stacking fault. For sample B, defects of the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epi-layer are confined into the low-temperature single $\text{In}_{0.4}\text{Ga}_{0.6}\text{As}$ buffer layer, without extending to the subsequent grown $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ epi-layer. Furthermore, the atoms will rearrange within the buffer layer through the annealing process, which is favorable for the subsequent epitaxy of the $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ layer. This achievement represents a simple but effective approach to achieve high-crystallinity $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ film on the Si substrates.

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