Transformation of the defect structure of InGaAs and InAlAs metamorphic buffer layers depending on indium concentration

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Abstract. A study of samples grown by molecular beam epitaxy using the technology of InₓAl₁₋ₓAs or InₓGa₁₋ₓAs metamorphic buffer layer formation on GaAs (001) substrate was performed by transmission electron microscopy. The 1 μm thick buffer layers with square-root dependence of In content on buffer layer thickness were studied in plan-view and cross-section geometries. The results demonstrate cascade step-wise relaxation of misfit strain along buffer layer thickness with the reduction of dislocation density to less than 10⁶ cm⁻² at the subsurface region. An inhomogeneous distribution of dislocations observed on plan-view TEM images is explained by overlap of split-level dislocation networks with different periods.

1. Introduction
Metamorphic buffer layers (MBL) have made it possible to obtain device structures with a high content of In on GaAs substrates that are cheaper and more available than InP substrates generally used for this purpose. The transition from the GaAs substrate to the active layer is conventionally accomplished by gradual change in the lattice constant along the MBL through layer composition alteration. Misfit strain arising in MBL because of the lattice mismatch relaxes by formation of crystalline structure defects, mainly dislocations. The specificity of such MBL is that the defects can generally remain inside the transition layer that allows one to achieve a low defect density in the overgrown active area. Sublinearly graded buffer layers were found to provide lowest misfit dislocation density and less residual strain as compared with step-wise or linearly graded ones [1].

The purpose of this work was to elucidate misfit dislocation network features in InₓAl₁₋ₓAs and InₓGa₁₋ₓAs MBL with square-root and linear In distribution.

2. Experiment
Samples were grown by molecular-beam epitaxy (MBE) on GaAs (001) substrates which were annealed before the MBL growth. A growth rate of 0.6 ML per second was kept constant during the whole growth process. Deposition of MBL was finished with a thin region with a constant indium fraction slightly reduced relative to the maximum. The thickness of the MBL was approximately 1 μm.

For samples A, B and C containing InₓAl₁₋ₓAs MBL two-stage growth was used: during the initial stage (up to 0.2 μm) the substrate temperature continuously lowered from 375 °C to 330 °C, at the last stage (after 0.2 μm) the growth was performed at a constant temperature of 330 °C. The fraction of indium was increasing according to the root dependence, starting from x=0.05 and ending with the maximum fraction of 0.8-0.9. The root dependence was realized by approximation with several linear segments of which the number was from 7 to 21 for different samples.
Samples D and E with In$_{x}$Ga$_{1-x}$As MBL were grown at the constant temperature from the range 380-400°C, growth rate being (0.6 - 0.8) ML per second. The In content was increasing linearly to a maximum fraction of 0.4. The details of the growth procedure can be found in [2,3]. Since transmission electron microscopy (TEM) is a suitable space-resolution tool to characterize the linear structural defects it has been used for the study of misfit dislocation array generated in InGaAs MBL. Cross-section and plane-view specimens for TEM study were prepared by a conventional technique including preliminary mechanical thinning and final ion milling. The specimens were investigated employing Philips EM420 and Jeol JEM-2100F microscopes using diffraction contrast imaging and selected area electron diffraction (SADP).

3. Results and discussion

Investigation of the samples with MBL was carried out by TEM in both cross-section and plan-view geometries.

3.1. Cross section

Fig. 1 demonstrates cross-sectional TEM images of the samples A, B and C with MBL of approximately equal thickness (about 1 µm). The samples slightly differ in the maximum In content (the maximum concentration of indium is 81%, 85% and 87% for A, B, C, respectively) and in number of linear segments approximating the root dependence of In content. The MBL extends from the GaAs substrate to the interface with devise structure which is represented as a thin dark line in the upper part of the images in Fig. 1. One more thin line of the dark contrast closer to the surface represents quantum well. The dislocations represented on the images as thin lines of dark contrast are predominantly contained within the bottom region of the MBL while the upper part of the MBL is almost free of defects. The multistage dislocation network at the MBL bottom region is known to necessarily form to relieve the mismatch strain arising due to growing In content. What stands out is nonuniform distribution of dislocations over the MBL thickness within the bottom region: they are concentrated at curved stripes separated by almost dislocation-free intervals.

![Figure 1 (a, b, c). 220 bright-field (110) cross-section TEM images of samples A (a), B (b), C (c)](image)

To monitor these alterations, the dislocation density was measured along the MBL thickness. The dislocation density was determined as total dislocation length divided by a selected volume, the TEM
lamella thickness being measured by means of convergent beam diffraction. In Fig. 2 the measured density of dislocations is plotted against the distance from the substrate-MBL interface for the samples A, B and C. As it can be seen, the dislocation density along the MBL thickness has local minima and maxima, while it decreases almost to zero at the upper part of MBL. As it also seen, the average dislocation density in the sample A is higher than that in the samples B and C.

![Figure 2. Distribution of Dislocation Density over the MBL thickness](image)

In addition, the relative lattice mismatch along ($\Delta a^\perp/a_{\text{sub}}$) and normal ($\Delta a^\parallel/a_{\text{sub}}$) to the growth direction was determined in dependence on the distance from the substrate-MBL interface by means of

![Figure 3 (a, b). Variation of relative lattice mismatch over the MBL thickness for samples A (a) and C (b): $\Delta a^\perp/a_{\text{sub}}$ (blue) and $\Delta a^\parallel/a_{\text{sub}}$ (red)](image)
measurements of corresponding reciprocal lattice vector length on SADP with the reference to GaAs substrate interplanar distances [4]. The results of relative lattice mismatch measurements for the samples A and C are shown in Figure 3.

The graphs in Fig. 3 show that the value of $\Delta a/a_{sub}$ at some regions becomes greater than $\Delta a/a_{sub}$, which indicates that the lattice there becomes elastically strained, i.e. generation of misfit dislocations is essentially suppressed, and elastic energy accumulates during the growth of this parts of MBL. When the elastic energy reaches a critical value, the intensive generation of mismatch dislocations happens that is reflected in that the components of relative lattice mismatch in both directions ($\Delta a/a_{sub}$ and $\Delta a/a_{sub}$) become equal to each other. These points are marked in Figure 3a as “jumps” in the dislocation formation process.

Thus, the nonuniformity of the contrast on the cross section TEM image is explained by cascade generation of mismatch dislocations due to stepwise relaxation of strain.

**Figure 4 (a, b, c).** 220 bright-field plane-view TEM images of the samples D (a) and E (b), and modeled moiré fringes (c).
3.2. Planar images
TEM plan-view images of samples D and E represented in Fig. 4 show dense misfit dislocation network. The network is seen to be irregular with alternating dislocation groupings and rarefactions. Such irregularity cannot be explained by the variation in the plastic relaxation extent (i.e. misfit strain variation) over the MBL growth surface. To elucidate the reason of dislocation groupings and rarefactions appearance on the plan-view TEM images we performed a simple simulation of projection of four overlaid square lattices with different periods. The result of the simulation is presented in Fig. 4c and seems to be similar to experimental TEM images. We can conclude that the observed irregularity in dislocation distribution on plan-view TEM images is apparent and occur as the result of translational moiré effect due to the presence of multistage dislocation network. The appearance of apparent dislocation groupings and rarefactions on the plan-view images of MBL allows us to conclude that the multistage dislocation network has somewhat dissimilar periods at different levels.

4. Conclusion
TEM study of 1 μm thick In_{x}Al_{1-x}As and In_{x}Ga_{1-x}As MBLs grown on GaAs (001) substrate with square-root and linear profile of In content was performed to characterize the misfit dislocation network. The obtained results demonstrate cascade step-wise generation of misfit dislocations with increasing MBL thickness yielding the reduction of dislocation density to less than 10^{-6} cm^{-2} at the MBL subsurface region. An inhomogeneous distribution of dislocations observed on plan-view TEM images is explained by overlap of split-level dislocation networks with different periods.

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