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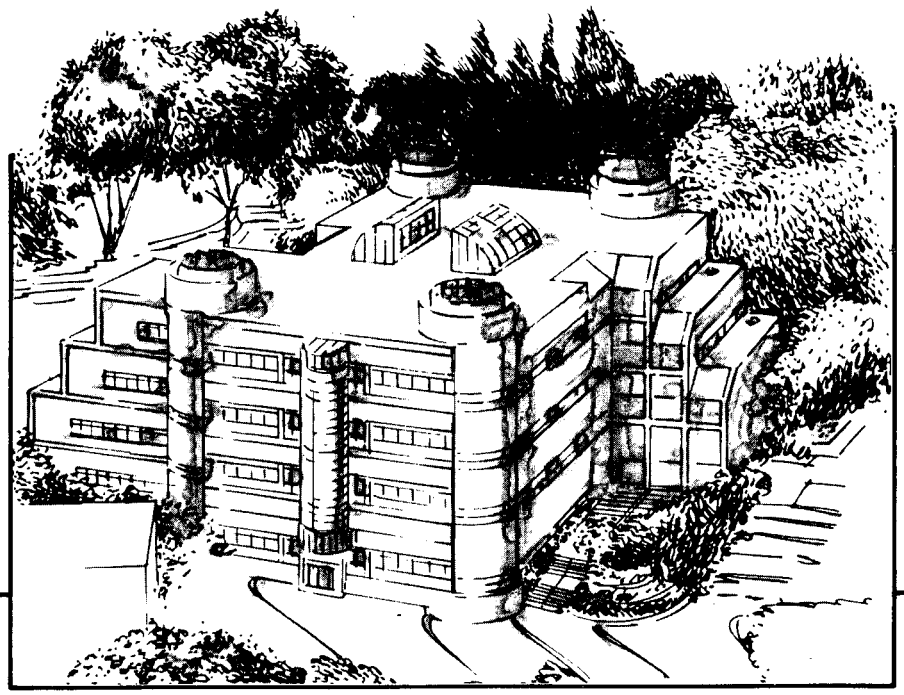

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STRAIN DISTRIBUTION IN HETEROLAYERS WITH LOW MISFIT AS REVEALED BY CONVERGENT BEAM ILLUMINATION METHODS

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ABSTRACT

Convergent beam electron diffraction (CBED) was applied to the local measurement of lattice parameter across a strained interface with small mismatch. GaAs layers grown at low temperature with excess As (with 0.15% misfit) on a GaAs substrate were chosen for these studies. Tetragonal distortion was detected in the layer up to 0.5 μm from the interface. With an increase of the layer thickness lowering of the symmetry of these CBED patterns was observed. This lowering of symmetry is most probably due to saturation of As solubility and the strain build into these layers.

I. INTRODUCTION

Convergent beam illumination methods were applied to the study of the lattice distortion within a layer with a small mismatch to the substrate. GaAs layers grown on [001] GaAs substrate at 195°C (called LT-GaAs layers) were chosen to these studies. These LT-GaAs layers are grown by molecular beam epitaxy (MBE) with excess As and are known to be As rich and show lattice expansion up to 0.15% [1].

TEM studies on these layers show that with increasing LT-layer thickness, specific defects called "pyramidal defects" are formed. These pyramidal defects are formed after the growth of specific thickness of perfect monocrystalline material and originate from nucleation of dislocations or stacking faults. The maximum thickness of the perfect material decreases drastically with decreasing growth temperature.

One explanation of this breaking of perfect crystallinity in Si and GaAs was given by Eglesham et al [2]. It was considered that breakdown of perfect crystallinity is an intrinsic feature of MBE growth at low temperature and to be due to increasing surface roughness built into the layer during the early stages of growth. However, for LT-GaAs, this might also depend upon changes in the As-rich stoichiometry of the growth front. Change in the localized growth direction from [001] to [011] with clearly visible [111] faceting observed in thick LT-GaAs layers was reported by us earlier [1]. However, the previously reported transition to amorphous growth [2] was never observed using our growth parameters.

An alternative explanation for the breakdown of perfect crystallinity may be strain buildup in the layer due to increasing excess of As responsible for the expansion of the lattice parameter [1]. Based on this assumption, only a specific layer thickness, called the "critical layer thickness (h_c)," can be grown for a given growth condition. Once this critical layer thickness is exceeded, misfit dislocations form at the surface that glide to the interface, relieving the misfit strain. Our previous experiment [1] shows that the LT GaAs epilayer thicknesses at which the onset of pyramidal defects occurs lies between the theoretical critical layer thicknesses (h_c) for pseudomorphic growth predicted by People and Bean [3] and by Matthews and Blakeslee [4]. Thus it is possible that the elastic strain incorporated in the LT GaAs layers as a result of the excess As is responsible for the defects formed in the layer.

II. EXPERIMENTAL

Convergent Beam Electron Diffraction (CBED) patterns were taken on four different samples. These four samples were grown under the same condition, with different LT-GaAs layer thicknesses. The samples with the larger (3.3 μm and 1.7 μm) thicknesses show formation of pyramidal defects (not shown for the lack of space) and the samples with the smallest layer thickness (1.4 μm and 0.9 μm) do not show these defects. These defects originate at a layer thickness of about 1.6 μm . CBED patterns were taken on cross-section samples prepared in [110] direction. These patterns were taken in many areas of the samples starting in the substrate far from the interface up to the top of the grown layer (or up to the area with pyramidal defects). The CBED patterns obtained in the substrate far from the interface were treated as the standard patterns and computer simulation varying the accelerating voltage allowed us to match the experimental patterns with calculated patterns. Usually, to match the pattern of the substrate, an accelerating voltage had to be changed for different samples. Instead of the nominal 200 keV, 201.1 to 201.5 keV was used. For such matched patterns, the indices to the HOLZ lines were determined.

In all cases the CBED patterns obtained in the interfacial areas had diffuse HOLZ lines from the planes almost perpendicular to the [001]-c axis, while the HOLZ lines from the planes almost parallel to the c axis remained sharp (Fig. 1a). This was true for the areas closest to the interface, and up to 0.06 μm on both sides of the interface.

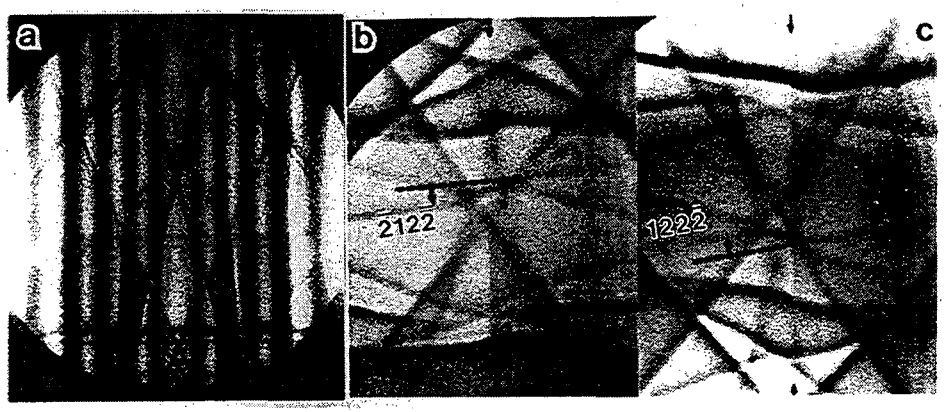

Fig. 1a). CBED pattern taken with [221] electron beam incidence at the interface. CBIM patterns: b) with the [510] incidence and c) [150] incidence direction, showing the shift of Kikuchi lines in opposite direction in these two equivalent projections.

The broadening of the HOLZ lines in the interfacial area suggests bending of the planes at the interface. To understand this behavior, two different CBIM patterns were obtained in the same interfacial area, with incidence directions of [510] and [150]. Very large bending of all HOLZ lines was observed across the interface. A shift of these lines in the layer was observed in the opposite direction, when a particular line is considered, such as $\bar{2}12\bar{2}$ in the [510] direction (Fig.1b) and an equivalent $122\bar{2}$ line in the [150] projection (Fig.1 c). Such a large shift cannot be expected from the slight lattice parameter change detected by x-ray studies [1]. In order to explain the line bending in convergent beam image (CBIM) surface relaxation of the thin TEM foil (described earlier by Eglesham [5]) needs to be taken into account. Bending of the planes along the [110] direction (parallel to the electron beam) is expected, since the thin foil is prepared in this direction. Details of this study is described elsewhere [6].

At a layer thickness more then 0.06 μm from the interface, all HOLZ lines regained their sharpness. A shift of some HOLZ lines was noticed when compared to the patterns obtained on the substrate. The question remains open as to what kind of lattice distortion is taking place and how uniform the distortion is across the layer. In order to find the difference between the layer and the substrate CBED patters were taken as well on imaging plates to increase sensitivity of this method. From the pattern taken on the GaAs substrate in [110] projection only one mirror

plane can be seen along [200] direction since (200) disc and ($\bar{2}00$) disc are different because they represent atomic planes of As and Ga (Fig. 2a). This mirror symmetry is lost when similar pattern was taken on the layer (Fig. 2b). This suggest lower symmetry of the layer compared to the substrate.

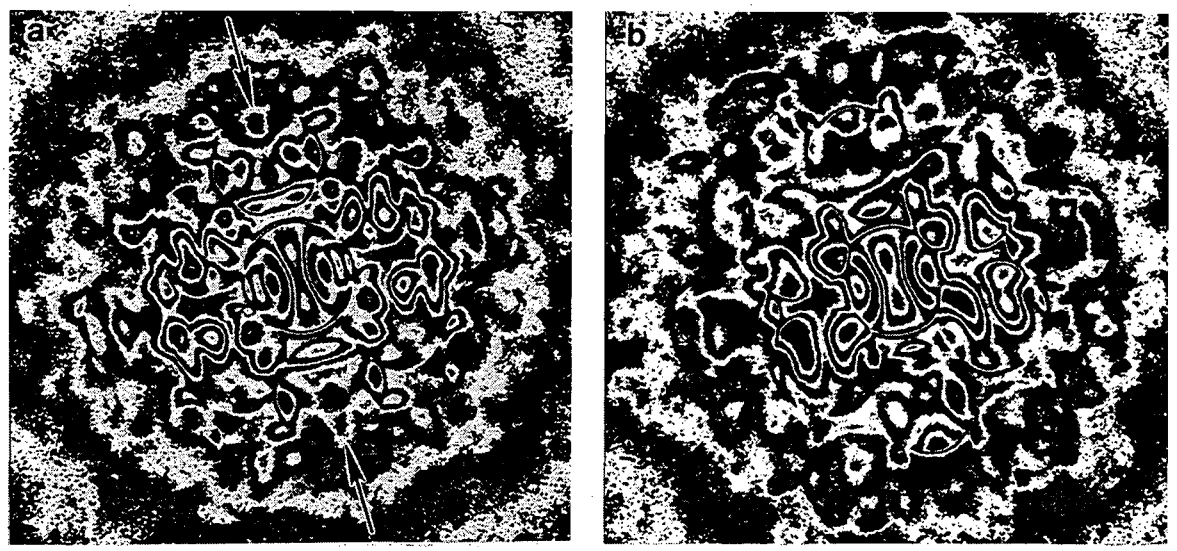

Fig. 2. CBED pattern taken with [110] electron beam incidence: a) on the substrate with a mirror symmetry along [200], b) on the layer - note loss of mirror symmetry.

To find out the distribution of strain in the layer CBED patterns were taken in two perpendicular directions [221] and [530] in many areas of the sample to find out the change of the lattice parameter. For layer thicknesses at 0.06 μm or more from the interface, lattice expansion was detected in both the [221] and [530] directions. The change in lattice parameter was noted as well for the direction close to [530] (exact orientation [0.869 0.495 0]), since the position of the cross of the $\bar{1}1\bar{1}\bar{3}$ and $\bar{1}113$ HOLZ lines changes when an electron beam was placed in the substrate (Fig. 3 a) and the layer (Fig. 3 b), respectively. The mirror symmetry was preserved in this pattern. This change in the cross position can be interpreted by a tetragonal lattice expansion ($a=b=a_s=0.5653$ nm and $c=0.5658$ nm), since the cross is formed by the planes inclined at near right angles to this axis. Therefore tetragonal distortion ($a = b = a_s$ and $c > a_s$) needs to be considered in this area of the sample. The same conclusion was obtained taking into account the symmetry of the [221] patterns.

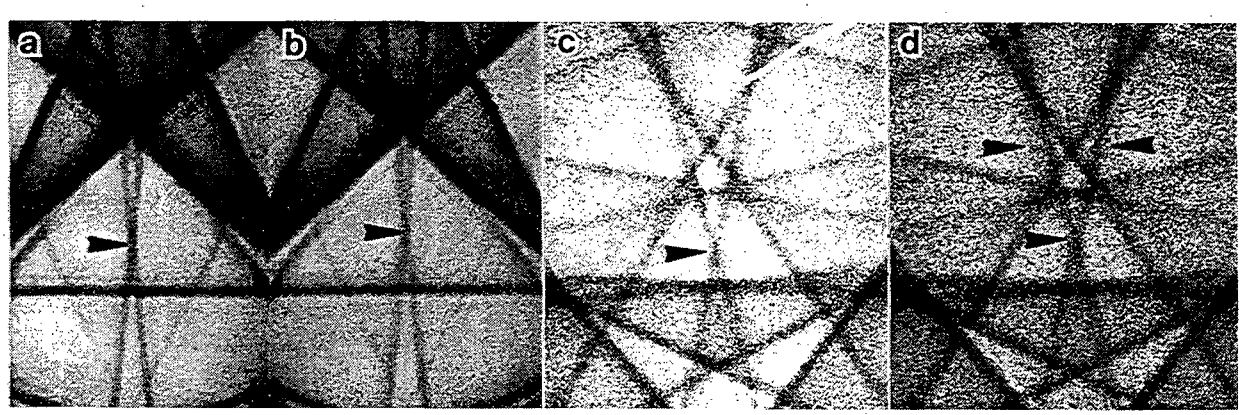

Fig. 3. CBED pattern taken near the [530] incidence a) on the substrate, b) on the layer showing the lattice parameter change; CBED patterns taken with the electron beam incidence slightly tilted from [221]; exact orientation [0.981 0.196 0]; c) on the substrate, d) on the layer. Note loss of the mirror symmetry in the last pattern.

For the larger layer thickness, some asymmetry in the HOLZ pattern was noticed for the

[221] incidence, with a clear loss of mirror symmetry parallel to the 220 lines. Breaking of the mirror symmetry was observed as well when the sample was tilted in the perpendicular direction to the [221] such as [0.981 0.196 0] shown in (Fig. 3 c, d). This broken symmetry was observed at layer thicknesses larger than 0.5 μm. It is not believed that pyramidal defects present in the top of the layer could influence the symmetry of these patterns. First pyramidal defects were formed at layer thickness larger than 1.6 μm; therefore the CBED patterns were taken only up to 1.4 μm
from the interface in order to avoid splitting of the particular HOLZ lines by these defects.The lack of mirror symmetry cannot be explained by cubic, tetragonal, hexagonal or rhomboedric symmetry. The highest crystal symmetry that can explain such a pattern is the orthorombic symmetry. Computer simulation of the arrangement of these lines gives a= 0.5653 $=a_s$, b=0.5658 nm (0.09 % change), and c=0.5662 nm (0.16% change) at a layer thickness of 0.6 μm from the interface. As one can see, this is only a slight distortion from tetragonal distortion, since the change of the b axis is very small. At a larger layer thickness from the interface a larger expansion in the b axis was observed for this sample. Such a change in the lattice parameter would lead to the formation of misfit dislocation. This would explain the fact that, at a certain layer thickness, pyramidal defects can form starting from misfit dislocations. Evidence for this mechanism includes dislocations and stacking faults found near the top of the crystalline layer (at the origin of pyramidal cores) that were obviously unable to glide down to the strained interface.

V. CONCLUSIONS

In this study it has been shown that LT-GaAs layers are strained. Tetragonal distortion was measured at a layer thickness up to 0.06 μm from the interface. Above 0.5 μm from the interface a lowering of the symmetry of the CBED pattern was observed. The calculated lattice parameter for this pattern is consistent with orthorombic distortion. It is not clear yet if these decreases in symmetry are artifacts of the TEM thin foil due to a surface relaxation in the direction parallel to the thin axis of the sample, as was described earlier by Eglesham [5] or if a gradual change in the lattice parameter is really taking place. One strong argument for gradual lattice parameter change is that reproducible results were obtained in four independent samples grown under the same condition, with the only difference in growth time. Since As accumulation on the LT-GaAs layer surface was detected in all samples with pyramidal defects [1] this suggest that the solubility of As in these samples became saturated at a certain layer thickness.

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