Journal of Electronic Materials, Vol. 22, No. 5, 1993

A Study of the Evolution Process of Antiphase Boundaries in GaAs on Si

S.I. MOLINA, G. ARAGÓN, and R. GARCÍA

Departamento de Química Inorgánica, Universidad de Cádiz, Apdo. 40, 11510
Puerto Real (Cadiz), Spain

Y. GONZÁLEZ, L. GONZÁLEZ, and F. BRIONES

Centro Nacional de Microelectrónica, CSIC, Serrano 144, 28006, Madrid, Spain

A study by high resolution electron microscopy and conventional transmission electron microscopy of the process of closure of antiphase boundaries (APB) in atomic layer molecular beam epitaxy (ALMBE) grown GaAs on silicon is reported. A parallelepipedical shape, closed at the top by another boundary with a semispheric shape, is proposed for the during growth suppressed APBs in GaAs epilayers. Antiphase boundaries are mostly located in {100} plans. Sixty degree dislocations are involved in the process of bending of APBs from {110} to {11 n} planes; this bending is the initial step which must take place to get a single domain by interaction of two APBs. The proposed shape for closed APBs is in good agreement with the quasi two-dimensional growth observed for GaAs grown on silicon by ALMBE.

Key words: ALMBE, antiphase boundaries, GaAs on silicon

INTRODUCTION

Various early works on antiphase boundaries (APBs) in III-V semiconducting materials with a sphalerite structure deal with the bulk distribution of domains,[1,2] the prediction of the crystallographic planes in which APBs appear,[3] and experimental methods to avoid them.[4,5] The more recent works deal with the following goals:

- To get antiphase-domain-free layers.[6–8]
- To establish what are the APB annihilation mechanisms.[9]

Structural studies of APBs by cross section and planar view transmission electron microscopy (TEM) have also been reported. These studies were done by high resolution electron microscopy (HREM)[10] or taking (002) dark field images.[11]

In this paper, we present HREM images ascribed to antiphase boundaries which mutually interact to further disappear. The analysis of such images allows us to propose a structure for the APBs' closure, on an atomic scale, in which the bending of an APB takes place.

EXPERIMENTAL

Growth of the Samples

The samples studied in this work are GaAs epilayers grown on silicon (001) substrates misoriented two degrees toward [110] direction. A 0.2 μm thick GaAs layer was firstly grown by atomic layer molecular beam epitaxy (ALMBE)[12] at substrate temperature T = 350°C, followed by 1 μm thick GaAs layer grown by conventional MBE ($T_s = 580°C$). By ALMBE, we find[13] that the nucleation of GaAs on silicon is closer to 2D mode than by a conventional low temperature MBE process. During growth, evolution of APBs was monitored by reflection high energy electron diffraction (RHEED) and reflectance difference (RD) techniques. We observe that a single domain GaAs growth front is achieved at a GaAs thickness less than 0.12 μm.

Reflectance difference is sensitive primarily to surface anisotropy induced by Ga-Ga dimers which are aligned along [110] direction in a single domain GaAs surface. On a GaAs layer grown on silicon with two types of domains, different surface areas will show mutually perpendicular Ga-Ga dimer orientations and the resulting RD signal amplitude will be reduced

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(Received September 25, 1992; revised February 26, 1993)

by a factor proportional to the relative difference between the surface areas of both domains.[14,15] In this way, RD provides quantitative information on the relative abundance of the antiphase domains in the GaAs growing layer. In particular, for the samples studied in this paper, we were able to assess that a single domain GaAs growth front was achieved at a GaAs thickness less than 120 nm.

A number of cross section and planar view transmission electron microscopy specimens have been prepared from 3 mm diameter discs ultrasonically cut from the epitaxially grown layers. The discs of cross-section specimens were mechanically thinned by grinding and dimpling, and finally were ion milled.

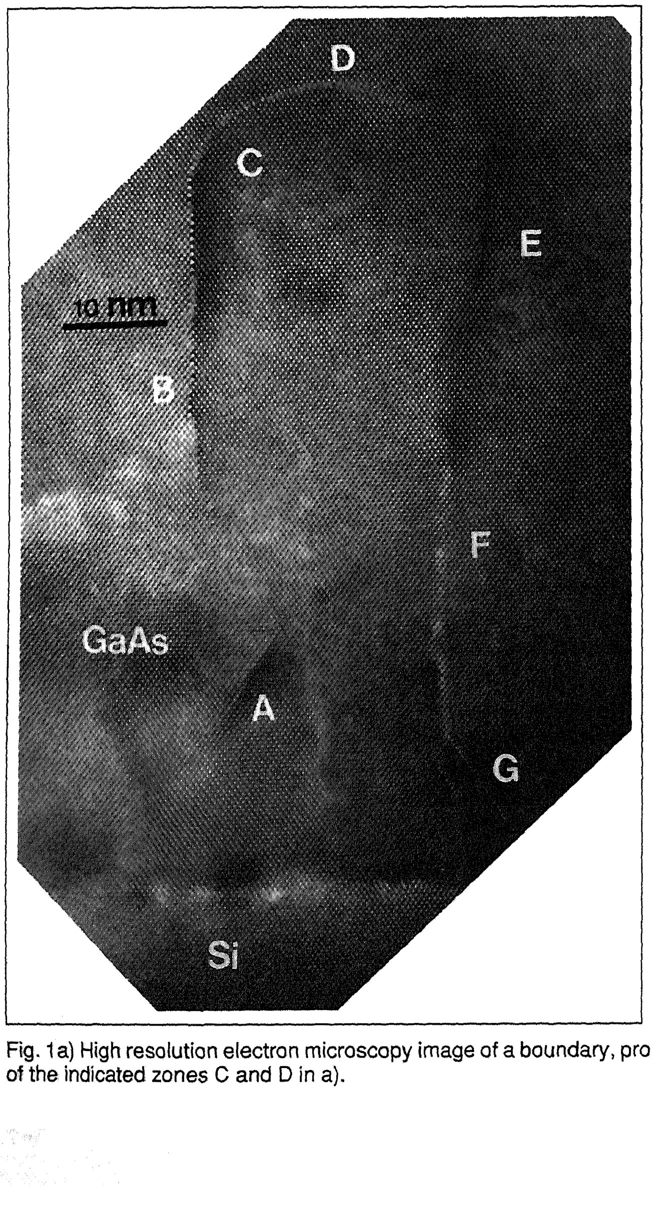
Method of Observation of the APBs by TEM

The procedure to locate an APB is as follows: a dark field image with a superlattice reflection is taken, resulting in a strong contrast in the regions in which APBs exist. Subsequently, a dark field with a fundamental reflection is obtained, leading to a zero contrast (kinematically forbidden reflection). The possible APBs will be located at the regions which show a strong contrast with a superlattice reflection and a faint contrast with an appropriate fundamental reflection. This faint contrast may be weak but not zero as double diffraction may occur.

The APBs have usually characteristic shapes, which help to distinguish them from other defects. Nevertheless, some cases might occur in which it would be complicated to decide if a certain contrast is actually due to an APB. In these cases, the method proposed by Edington[16] of applying a two beam condition is used. The expected TEM image of an APB under two beam conditions consists of a group of alternated white and black fringes which are parallel to the direction [uvw] of intersection of the APB plane with the surface of the material film in which that APB is placed. This TEM image has some typical features.

Once an APB has been located, it can be studied by HREM. However, an HREM image does not yield by itself useful enough information to describe the structure of the APB unless some requirements are fulfilled:

- The section of the APB should be prepared in such a way that the electron beam incidence direction is contained in the APB plane. If not, the APB is projected on a geometric region which is not a simple line, making more difficult the interpretation of the observed contrast.
- In order to obtain specific information about the APBs, the electron-transparent specimen thickness and the defocus conditions have to be suitable to create a HREM image contrast which differs from that corresponding to a perfect crystal. Some HREM image simulations[17] exist in which it is clearly shown that the specimen



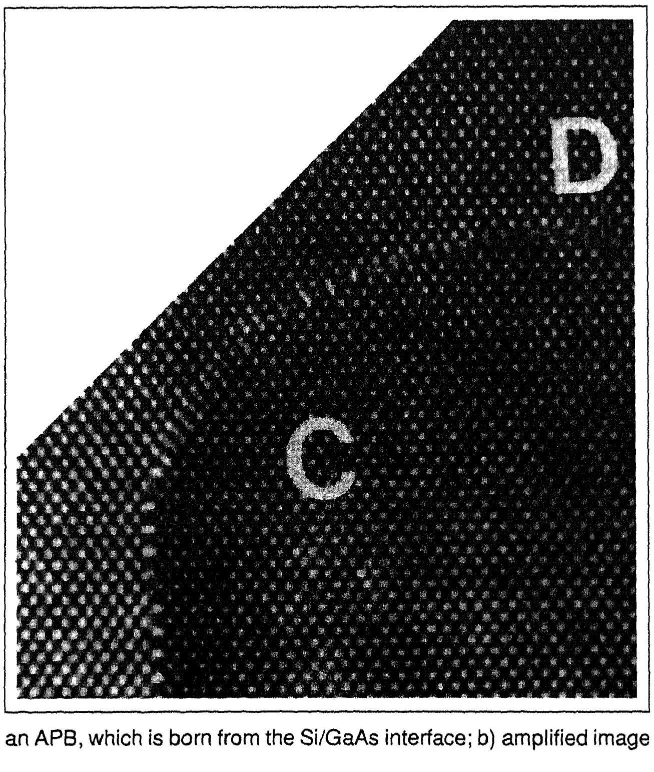


Fig. 1 a) High resolution electron microscopy image of a boundary, probably an APB, which is born from the Si/GaAs interface; b) amplified image of the indicated zones C and D in a).

thickness range which leads to different contrasts for an APB and for a perfect crystal is very narrow.

The HREM experimental results presented in this paper have been obtained using a transmission electron microscope JEOL 2000 EX (200 kV, top-entry, C_s = 0.7 mm). The material was oriented with the zone axis [110] parallel to the incident electron beam. The objective lens aperture allowed for the interference of seven beams. A transmission electron microscope JEOL 1200 EX was used for carrying out the contrast diffraction work with planar view prepared specimens.

RESULTS

Description of APBs in ALMBE Grown GaAs on Silicon

A number of HREM images have been obtained using the above mentioned procedure. Figure 1 shows one of these images which is particularly appropriate because the two previously mentioned requirements for obtaining useful images are fulfilled. Two APBs appear which bend at a *certain distance from the* Si/GaAs interface. As a consequence of this bending of the boundaries, one of the two possible types of domains is confined while the other becomes the unique domain as the growth proceeds. The contrast with the reversed U shape in this figure is interpreted as a transverse section of an APB with a parallelepipedical shape with curved corners, closed at the top by another boundary with a more or less semispheric shape. In Fig. 2, we show schematic drawings of one of these suppressed APBs as they should appear under different conditions (cross-section, planar view,...).

In Fig. 3, we show a planar view TEM image of APBs. Notice the quasi-square shapes which are similar to the proposed ideal shape schematized in Fig. 2a.

Although the proposed APB shape, as shown in Fig. 2a, is an ideal case, real APBs are in fact quite similar. However, deviations to this ideal case are evident (see Fig. 1). In the following, we will make a detailed description and comments on some features of the HREM image shown in Fig. 1:

- A spotless contrast of an APB for a certain plane is not observed in some regions which are placed near the GaAs/Si interface. This occurs, for example, in region labeled A. This is explained supposing that the electron incidence direction is not contained in the plane of the APB or that the APB plane is not unique. In fact, this happens for the curved corners regions of theabove proposed boundary (Fig. 2).
- The contrast is located, for the remaining regions of the boundary (B-F), in a region with a width smaller than 3 nm. This means that the APBs are located in planes which contain the electron incidence direction or that the angle among these planes and the incident electron beam direction is small (less than approximately 17 degrees). This maximum angle can be estimated as follows: the specimen thickness is about 10 nm. If the projected APB plane width is assumed to be equal to the inclined APBs contrast width, the angle can be estimated as arctan (3/10) = 16.7 degrees.

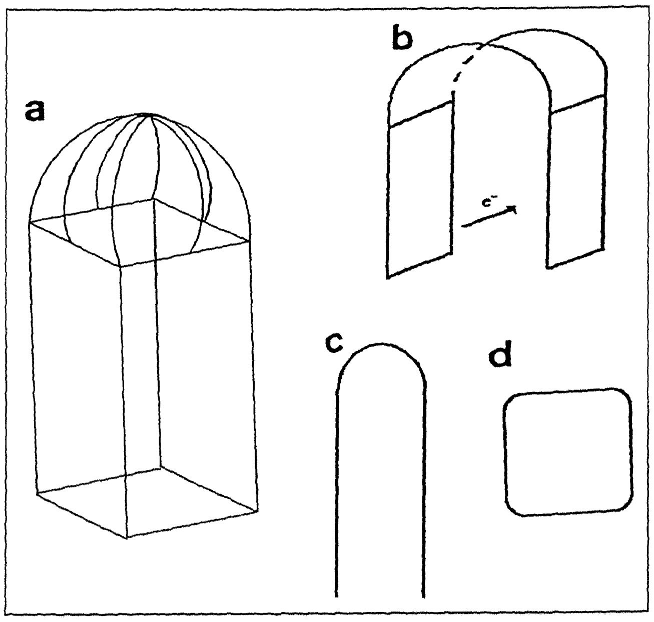


Fig. 2. Model form proposed for closed APBs. a) 3D representation, b) as the APB would appear in electron-transparent specimen prepared for a cross-section study, c) cross-section, and d) planar view.

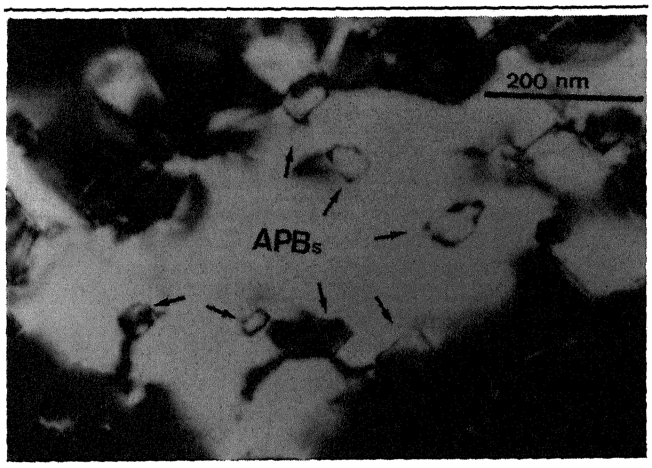


Fig. 3. Planar view TEM image. Antiphase boundaries are indicated by arrows.

- Interesting enough is the assessment of the most numerous APB planes. For some regions, as it is region labeled B, these planes are of {110} type. For other regions (E and F) the presence of APBs in {110} planes should be considered although the HREM image seems to be similar to that of a perfect crystal.[17] However, the APBs are located in planes with orientations which differ from {110}, in the regions labeled C and D, where the boundary is observed along {111} and {11 n} (n > 1) planes.

These results seem to confirm the work by Petroff[3]

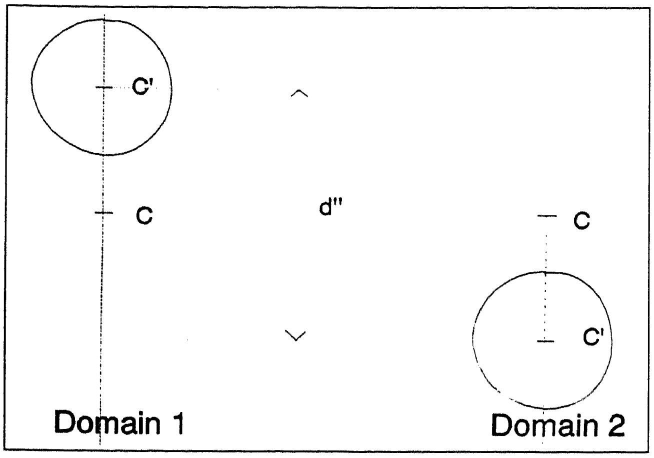


Fig. 4. Contrast distribution of contrasts in the two domans for both sides of an APB; d″ distance, measured in the direction [001], which a bright spot has been shifted from domain 1 up to domain 2.

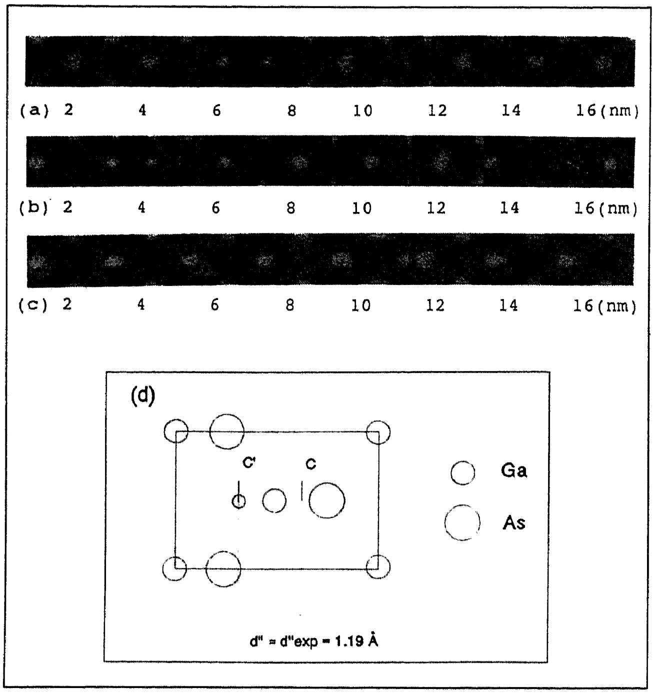


Fig. 5. GaAs simulated HREM images for several specimen thicknesses (t:2–16 nm), for different defocus values (nm): a)f_{Sch}–30, b)f_{Sch}; c)f_{Sch} + 30, d) scheme of the contrast disposition in the simulated image for t = 12 nm, f_{Sch}.

concerning the relative energetic stability of the planes in which APBs exist: it is energetically more probable for an APB to exist in a {110} than in a {111} plane. This is clearly observed in region B, and is one more reason for assuming that the APBs are in {110} planes in the E and F regions. Under these considerations, we can establish that about 60% of the boundary (regions B, E, and F) will be in {110} planes.

Several nonuniformily arranged dislocations are found along the boundary. For the case of the APB shown in Fig. 1, although no dislocations appear in a lateral of the boundary (regions E and F), some dislocations can be observed in the opposite lateral, though they are low in number. However, more dislocations are found in the boundary closure region (regions C and D).

An enlargement of the C-D region is shown in Fig. 1b. It can be observed how a 60° dislocation (or one with a very similar structure) is responsible for the change of direction in the boundary from a {110} plane up to a {111} plane.

Determination of the Existence of {110} APBs Using HREM Images

The HREM image for the [110] zone axis of GaAs consists, for a great range of conditions, of some bright spots which are associated with a dumbell of columns of projected atoms. The center of each spot does not have to coincide with the center of each dumbell. The polarity for the two domains in both sides of an APB is opposite. If a spot associated with a dumbell does not coincide with the center of the dumbell, it will be seen that the spots are shifted with respect to the dumbells as it is indicated in Fig 4.

The distance that a bright spot has been shifted from domain 1 up to domain 2, measured in a <111> direction can be measured using a HREM image of an APB, and d″ , as defined in Fig. 4, can be easily calculated from that measured distance.

The boundary appearing on Fig. 1 is located in a {110} plane for region G where d″ is equal to 2.38Å. This means that the center of a spot near the dumbell, in the direction [001], will be shifted 1.19Å from the center of the dumbell. The experimentally observed off-set in the HREM image for this region takes place for a specimen thickness of 12 nm and under the Scherzer defocus, as has been deduced from an analysis of simulated images (see Fig. 5).

DISCUSSION

As we explained before in this paper, the GaAs on silicon layers grown by ALMBE were in-situ characterized by RD which is a technique sensitive to the superficial anisotropy induced by Ga-Ga dimers and also allows for the monitoring of the domain concentration evolution.[14] A detailed description about the use of this technique for studying APBs has been given by Y. González et al.[15] Regardless of the growth conditions, a general behavior is observed for the domain evolution process in MBE and ALMBE grown layers. This process is characterized by two steps: 1) a process in which a fast decrease of one of the two possible types of domains takes place, up to the growth of approximately 50 nm of GaAs, followed by 2) a lower rate suppression process up to the total elimination of one domain type. The step distribution on the silicon starting surface as well as the growth conditions have a small influence on the kinetics during the first step. In particular, the APBs suppression process is faster when the layers are grown at low temperature by conventional MBE in relation to the ALMBE grown layers.

These results show that the domain evolution process is operative at the onset of growth: small antiphase domains will close faster than larger ones, making

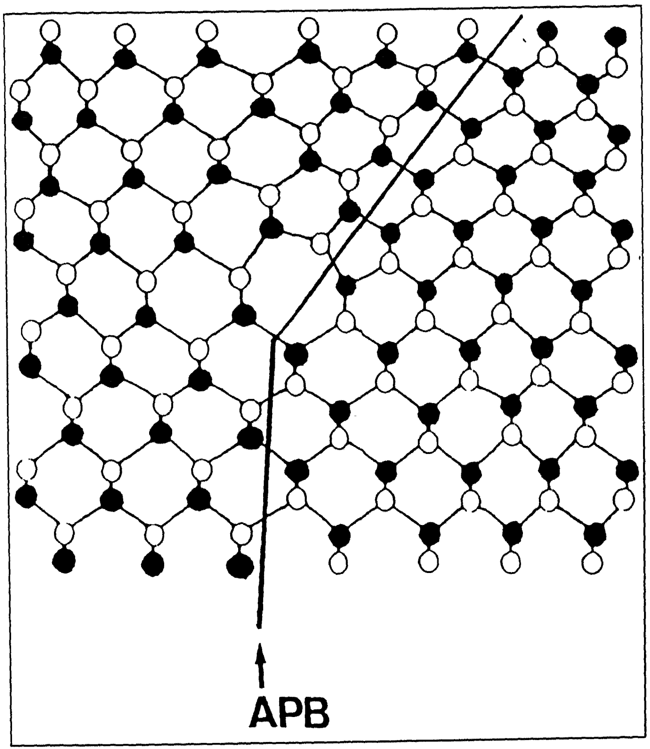


Fig. 6. Structure proposed to explain the bending of an APB.

the process less active when the domains are larger than, say 50 nm, or the boundaries are separated further than this distance.

It has also been suggested[16] that the closure of APBs could be related to the mechanism of lattice relaxation. This should not be discarded as some dislocations have been found along the boundary and in the closure zone. The presence of a dislocation could represent an activation for the APBs' folding process, finally leading to the closure of that APB, which is a lower energy state (perfect crystal state).

The structure shown in Fig. 6 is proposed to explain the bending process of APBs due to the contribution of a 60° dislocation. This structure shows that a dislocation of this type can be responsible for the bending of an APB as it has experimentally been observed. Antiphase boundaries suffer further bending processes up to be contained within the (001) growth plane and the disappearance of a type of domain takes place by interaction of two APBs as is schematically shown on Fig. 7.

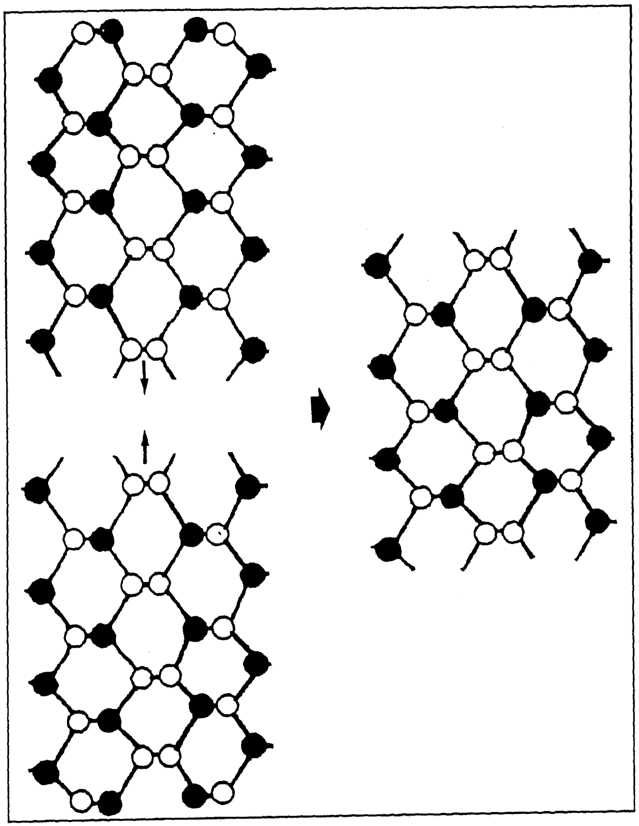


Fig. 7. One domain disappears from the surface after interaction of two APBs on (001) plane.

As we discussed in a previous work[13] we have demonstrated that the growth of GaAs layers on silicon (001) by ALMBE at low temperature is quasi two dimensional. In the following, we will describe the relation between the characteristics of this growth process and the observed structure of confined APBs, as well as the differences with the APBs evolution observed for GaAs layers grown on silicon by conventional MBE.

The presence of APBs running along {110} planes from the onset of growth in GaAs grown on silicon by ALMBE is reasonable in view of the quasi two dimensional growth mode. In this way, during layer by layer growth by ALMBE, the GaAs antiphase boundaries, initially coincident with the existing steps in [110] direction of the misoriented silicon (001) substrate surface, would continue propagating along the growth direction [001] until they are bent and eventually a couple of them interact. As a consequence of this process, one of the types of domains is confined while the other survives and is enlarged as growth proceeds.

In materials grown by conventional MBE, APBs initially on {110} planes appear macroscopically to fall on {111} planes; this was explained on the basis of the 3D growth produced in MBE grown materials.[10] The faster closure produced in MBE grown layers, compared to ALMBE,[14] could be explained by the formation of triangular APBs after two {111} planes collide as opposed to the more 2D growth[13] in the initial stages of the ALMBE grown layers. However, if the proposed closure mechanism is operative also for a conventional MBE growth, the slower closure process for ALMBE growth will be explained because the more 2D growth mode, the less important[18] is the role of 60° dislocation in the strain relaxation process, and these dislocations have been observed to be implied in the APBs closure process.

CONCLUSIONS

Antiphase boundaries in GaAs layers grown on silicon by ALMBE show a characteristic shape. They are parallelly disposed to the growth direction, and they bend to interaction among them. The bending consists of a change of the plane of the APB, from a {110} plane to a {111} plane, and afterward to other {11 n} planes (n > 1). This bending is associated to the presence of a dislocation with its line contained in the APB plane; a structure has been proposed to describe the bending of this type of boundary.

ACKNOWLEDGMENTS

This work has been supported by the Comisión Interministerial de Ciencia y Tecnología, CICYT, Project MAT 1205/91, and by the Junta de Andalucía, under the group 6020. This work was carried out at the Electron Microscopy Facilities of the University of Cádiz.

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