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Experimental evidence of the structure of annihilation of antiphase boundaries in GaAs on Si

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A high-resolution electron microscopy (HREM) study on antiphase boundaries in GaAs grown on Si is presented. HREM images of two close antiphase boundaries appearing mainly on the {110} planes which abruptly disappear suggest some ideas on the mechanisms of annihilation of these defects.

The antiphase boundaries (APBs) are defects which appear when a failure in the sequence of occupation of atomic planes is produced. These defects are found, as a particular case, in semiconductor heterostructures in which the epilayer is a polar material and the substrate is a non-polar material [1].

A special example of these heterostructures is the GaAs/Si system, especially interesting for its technological relevance. In this system, GaAs antiphase domains (regions between antiphase boundaries) could be avoided by growing on an atomically flat, perfect (001) surface if the very first layer is formed by either Ga or As atoms. However, any real (001) surface will always exhibit steps. Again no APBs would be expected if the surface steps are two atomic layers high ($\frac{1}{2}a_0$) where the sublattice allocations of Ga or As at both sides of the step are coincident.

Nevertheless, experimental results [2] have shown that antiphase boundaries (detrimental to the electrical performance of electronic devices) can be effectively suppressed by growing on slightly misorientated (001) substrates, even though they present a high surface density of monoatomic steps ($\frac{1}{4}a_0$). In this case the initially double-domain GaAs surface progressively evolves into a single-domain growth front.

In a previous work [3,4], we demonstrated that the APB annihilation process starts at the onset of growth and is thickness dependent. A short distance of about 1000 Å from the GaAs/Si interface is sufficient for achieving a single-domain growth front. We could assess as well a certain dependence of this process on growth conditions and step distribution on the Si starting surface. However, a clear understanding of the mechanisms operative in the suppression of antiphase domain remains unknown at present.

Transmission electron microscopy (TEM, HREM, CBED) techniques can be used for structural characterization of APBs. These techniques are the most suitable for this problem because of their high spatial resolution. CBED and conventional TEM [5,6] are more appropriate than HREM when the localization of many APBs is pursued. On the other hand, HREM is the ideal technique when the main aim is to study atomic structures and mechanisms associated with the annihilation of the APBs.

In this work we present experimental evidence, obtained by HREM, of the structure of closure of APBs in GaAs layers grown by atomic layer molecular beam epitaxy (ALMBE) on Si(001), 2° off towards [110] substrates. The samples consisted of a 0.2 μm thick GaAs layer grown by ALMBE at substrate temperature $T_s = 350°C$, followed by 1 μm thick GaAs layer grown by conventional MBE ($T_s = 580°C$). During growth, evolution of APBs was monitored by reflectance difference spectroscopy [3], observing that a single-domain GaAs growth front was achieved at a GaAs thickness less than 0.12 μm.

The procedure used to analyze the possible regions containing some APBs was as follows: (1) A conventional TEM study was done in order to localize the APBs; these defects must show a strong contrast when they are imaged with superlattice reflections of the sphalerite structure ($(hkl)=(002)$), while faint contrast is observed when certain fundamental reflections are used [7]. (2) Once the APB is localized, a cross-sectional HREM study (incident electron beam parallel to the zone axis [110]) was done. A JEOL 2000 EX top entry electron microscope (200 kV, structural resolution = 2.1 Å) has been used for this HREM study.

Fig. 1 shows a HREM image corresponding to one of these APBs which is born at the interface GaAs/Si and is suppressed at a distance of 57.6 nm from this interface. In a first approach, the APB shape suggested by the obtained cross-sectional HREM images, in agreement with other planar view studies, could be fitted to a rectangular prism with curved corners ending in a semisphere.

A closer observation of the HREM image reproduced in fig. 1 shows that the lateral faces of the APB run along {110} planes. The peculiar contrast of an APB, so different from that corresponding to a perfect crystal, is not observed in the regions labelled E and F. This could be explained by the many different imaging conditions (defocus, specimen thickness, etc.) that occur over the APB HREM image [8]. Some dislocations have also been found along the boundary, especially in the regions C and D. The extra planes of these dislocations are indicated with arrows (see fig. 2). Due to the existence or the appearance of a dislocation, the boundary changes its direction, firstly from {110} to {111}, and afterwards to another plane, $\{11n\}$ $(n>1)$.

Finally, the hypothesis of the presence of APBs running along {110} planes could be reasonable in view of the two-dimensional growth mode of GaAs on Si(001) by ALMBE at $T_s \approx 350°C$ [9]. The GaAs antiphase boundaries initially coincident with the existing steps in the [110] direction of the misoriented Si(001) substrate surface, would continue

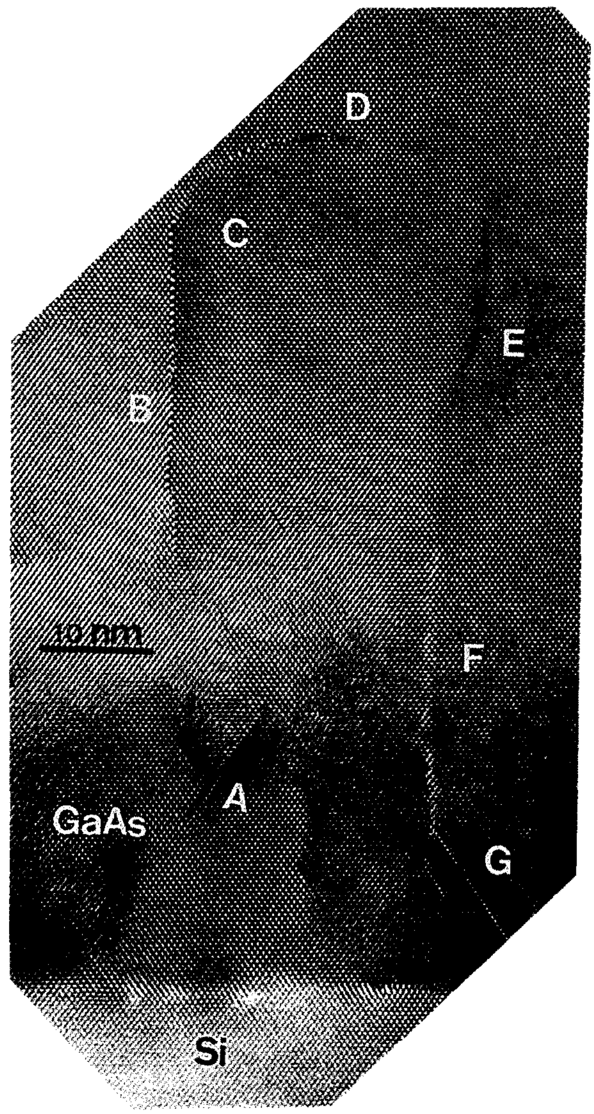

Fig. 1. HREM image of a region near the interface GaAs/Si. The structure of annihilation of a possible antiphase boundary which is born at the interface can be seen.

propagating along the growth direction [001] during layer-by-layer growth by ALMBE.

However, experimental evidence [3,4] suggests that domains annihilate linearly with thickness achieving a single domain growth front approximately 0.1 μm away from the interface, independently of growth kinetics (MBE and ALMBE). This implies that a certain dependence exists between the

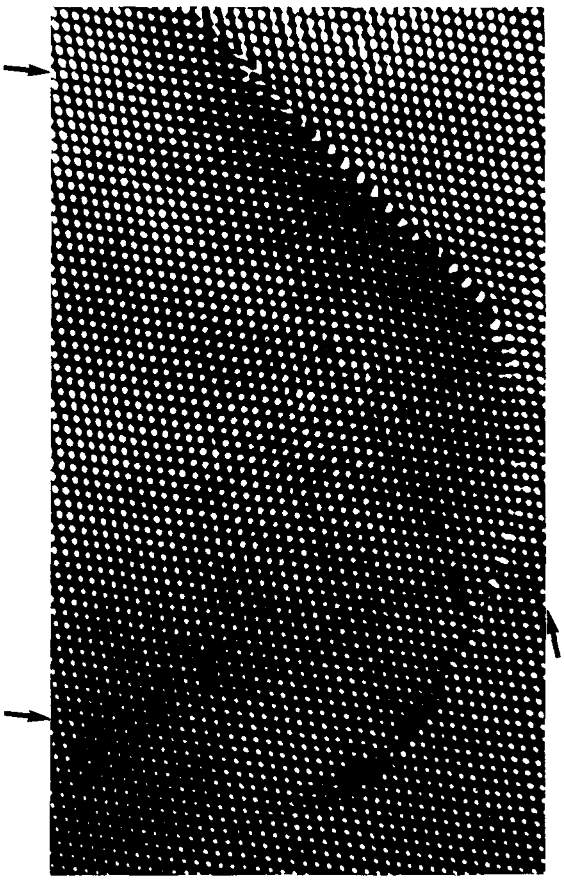

Fig. 2. Amplified image from fig. 1. The arrows indicate the extra planes from each dislocation found in this region of the boundary.

grown thickness at which domains annihilate and the lateral size (related to terrace size of distance between steps on the original Si surface). This dependence could be related to the mutual interaction energy between the boundaries or the surface energy of the domains (small domains annihilate earlier than large domains).

In summary, experimental evidence, obtained by HREM, of the structure of closure of APBs in heteroepitaxial ALMBE grown GaAs/Si systems is shown. The abrupt disappearance of the APBs suggests some ideas on the mechanism of annihilation of these defects.

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