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GRAIN BOUNDARIES AND ANTIPHASE BOUNDARIES IN GaAs

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ABSTRACT

Bicrystals of GaAs with a predetermined orientation relationships between the grains have been produced by growing GaAs epilayers on substrates cut from Czochralski-grown germanium bicrystals. Grain boundaries have also been generated in GaAs epilayers grown on (110) Ge substrate. In this report, an extensive study of such interfaces is illustrated by a transmission electron microscopy (TEM) study of the atomic structure of first-, second- and third-order twin boundaries. Antiphase boundaries (APBs) have also been produced in GaAs epilayers grown epitactically on Ge substrates. Both the structure of these interfaces and the interactions of the APBs with grain boundaries and lattice dislocations have been examined using TEM.

INTRODUCTION

When two crystals join at a certain misorientation angle, the grain boundary so formed tends to lie parallel to certain well-defined crystallographic planes. In many cases, these planes can be predicted using the CSL model; crystallographic planes containing a high density of coincident lattice sites appear to be favored as boundary planes. Randomly oriented grain boundaries are then commonly observed to facet parallel to these low-index planes.

The $\Sigma=3n$ twin boundaries in diamond-cubic materials are perhaps the most extensively analyzed class of interfaces; it is clearly interesting to compare the structure of these interfaces with those observed in III-V compounds with the sphalerite (zinc-blende) structure. Kohn [1] proposed atomic structure models for both the $\Sigma=3$ and the $\Sigma=9$ grain boundaries of a diamond-cubic crystal; the models assumed that a periodic array of atomic steps were present to produce the required boundary plane. Hornstra [2,3] extended this analysis and proposed atomic models for symmetrical grain boundaries in germanium in which the two grains are related by a rotation about either a $\langle 110 \rangle$ axis or a $\langle 001 \rangle$ axis. These models have generally been supported by experimental studies [4,5]. In materials with a sphalerite structure, the structure can be changed, without necessarily translating or rotating the lattice, by reversing the polarity of the crystal. Therefore, there are two possible relationships between the grains on either side of the interface for any given boundary in materials with diamond structure. These two structures can actually be interchanged by a rotation of one grain relative to the other of 180° about a $\langle 110 \rangle$ axis. In Si, for example, a 2-fold axis is parallel to the $\langle 110 \rangle$ axis; a mirror plane is normal to the same axis, thus giving the inversion symmetry: $2/m$. The polarity of each grain can be determined using the dynamical coupling effect of HOLZ reflections on (200) type convergent beam disks [7-10]. The atomic structure of the $\Sigma=5/[001]$ grain boundary and of low-angle grain boundaries in GaAs have also been extensively studied [11]. However, the present report will be limited to illustrations of the analysis of the atomic configurations of the $\Sigma=3$ and $\Sigma=9$ grain boundaries.

When a GaAs epilayer is grown on a (001) Ge surface, antiphase domains are expected to be produced since the polar material is growing on a non-polar material [12,13]. An antiphase boundary (APB) is a planar defect across which anti-site bonding takes place. This boundary can be expected to have a local displacement-field due to the different bond lengths between like (Ga-Ga, As-As) and unlike (Ga-As) atoms. This anti-site bonding may also influence the electrical properties of the epilayer. Both the electrical characteristics of APBs and their associated displacement-field may cause them to interact strongly with misfit dislocations, heterojunctions and grain boundaries. Illustrations of such interactions examined using TEM using flat-on and cross-section specimens are also illustrated in this paper.

EXPERIMENTAL PROCEDURE

A $\Sigma=3$, $\langle 110 \rangle$ bicrystal of GaAs was produced by growing undoped GaAs epilayers on a Ge bicrystal in a low-pressure organometallic vapor-phase epitaxy (OMVPE) system [14]. GaAs- $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ heterostructures were also grown on a (001) Ge surface so as to study the interaction of APBs with both misfit dislocations and heterojunctions. Flat-on TEM specimens were prepared by cutting 3-mm-diameter disks which were then mechanically polished from the Ge-substrate side and thinned from the same side in an ion miller using 4 kV Ar^+ . Cross-section specimens were prepared in the usual way, although the sample was cut, rather than cleaved, to give the required orientation. The cut slices were glued together so that the required low-index poles of the two pieces were parallel to one another. The samples were mechanically polished and ion-milled as for the flat-on specimens. The interface structures were studied using JEOL 1200EX and 4000EX electron microscopes.

RESULTS AND DISCUSSION

1.1 $\Sigma=3$ Coherent twin boundary

An image of a $\Sigma=3$ boundary and the corresponding diffraction pattern are illustrated in Fig.1a. The diffraction pattern indicates the relationship between the grains on either side of the boundary; the growth surface is $\{110\}$ and the boundary plane is parallel to $\{111\}$. Sharp streaks are visible in the diffraction pattern which result from the boundary structure [15]. The average grain boundary plane was chosen to be $\{111\}$ although, as shown in Fig.1a, faceting does occur, in particular, parallel to $\{112\}/\{112\}$ and $\{122\}/\{100\}$ planes. The details of the atomic structure of the $\{112\}/\{112\}$ boundary are described in section 1.2. Through-focal-series of high-resolution electron images were recorded from the same boundary. Fig.1b shows a typical HREM image which was recorded at a specimen thickness of less than 165 Å. The thickness was deduced from the intensity change produced by amplitude oscillation of the transmitted beam. Computer image simulation was carried out for a wide range of defocus values and specimen thicknesses. The polarity of each grain was determined by examining the dynamical coupling effect of HOLZ reflections on (200) convergent-beam disks; the "dark-cross" and the "bright-cross" HOLZ lines indicate the relative position of gallium and arsenic in the lattice. The comparison of the high-resolution micrographs with the simulated images and the determination of the polarity of each grain shows that the observed $\Sigma=3$ tilt boundary is a coherent twin boundary across which no anti-site bonds (Ga-Ga or As-As) exist. One model of the atomic configuration for this boundary, consistent with the above experimental results, is suggested in Fig.1c.

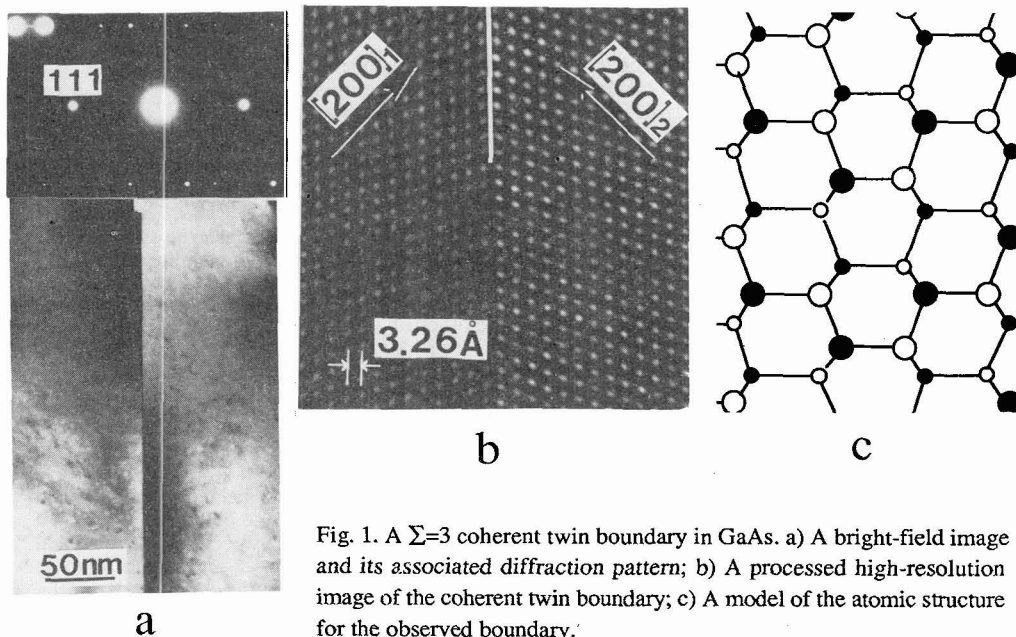


Fig. 1. A $\Sigma=3$ coherent twin boundary in GaAs. a) A bright-field image and its associated diffraction pattern; b) A processed high-resolution image of the coherent twin boundary; c) A model of the atomic structure for the observed boundary.

1.2. $\Sigma=3$ twin boundary faceting on the (112)/(112) plane

Many microtwins are produced when GaAs epilayers are grown on (110) Ge substrates [16]. These microtwins actually provide model examples of first-, second-, and third-order twin boundaries with a variety of grain-boundary planes. A high-resolution image obtained from one of these microtwins is illustrated in Fig.2a. First-order twin boundaries, $\{111\}_A/\{111\}_B$, $\{112\}_A/\{112\}_B$, $\{122\}_A/\{100\}_C$, $\{111\}_A/\{115\}_C$, and a second-order twin boundary, $\{111\}_B/\{115\}_C$ are observed. A magnified view of the image of the $\{112\}_A/\{112\}_B$ segment is illustrated in Fig.2b. Two structural units of this boundary are indicated with arrows. No lattice translation is present along this facet. The microtwins are located in the first extinction distances of the 000 beam. An optical diffractogram obtained from the amorphous region confirmed that the image was recorded near the Scherzer defocus of the objective lens. Lattice images have been simulated for a symmetrical (112)/(112) twin boundary for a range of a series of defocus values near Scherzer focus and for specimen thicknesses up to 135Å. A selection of these simulated images is illustrated in Fig.2c. From a comparison of the high-resolution images with the simulated images, the bright spots of the micrograph correspond to the channel while the dark spots correspond to atomic columns consisting of gallium and arsenic atoms in a (110) projection. This analysis is confirmed by the observation that the bright spots lie along the mirror plane of the coherent first-order twin boundary [17,18]. The atomic arrangement of this boundary is suggested in Fig.2d, assuming that the coherent twin boundary does not contain any anti-site bonds across the boundary. Computer image simulation has been carried out for the case in which the polarity of one grain is reversed, but the contrast change is too small in GaAs to be observed [18].

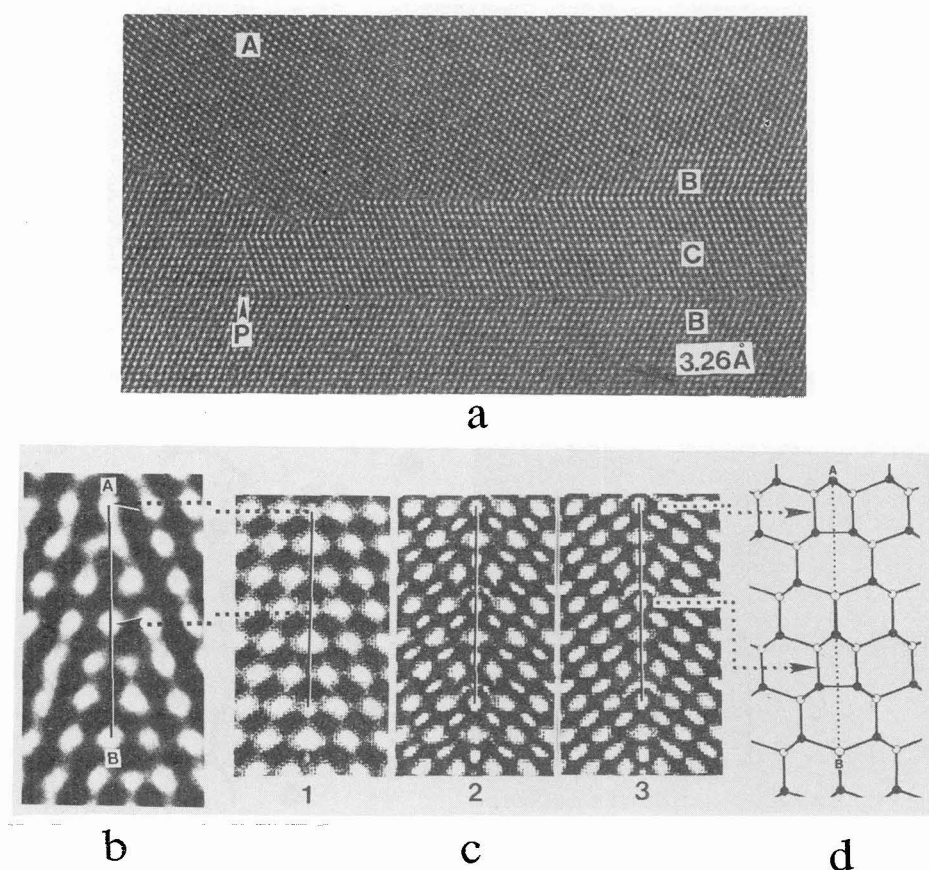


Fig. 2 A $\Sigma=3$, (112)/(112), (110) Lateral-Twin Boundary. a) A high-resolution electron micrograph of microtwins in a GaAs epilayer; b) A magnified view of (a) showing the (112)/(112), $\langle 110 \rangle$ facet; c) Computer simulated images: i) $\Delta f=-482.0\text{\AA}$, $t=20.0\text{\AA}$; ii) $\Delta f=-482.0\text{\AA}$, $t=80.0\text{\AA}$; iii) $\Delta f=-482.0\text{\AA}$, $t=119.9\text{\AA}$ d) A model of the atomic configuration.

1.3. $\Sigma=9$ (111)/(115), (110) Second-Order Twin boundary

Two $\Sigma=3$ coherent twin boundaries can interact with one another to produce a third boundary as illustrated in Fig.3a. This boundary facets parallel to particular crystallographic planes, including {111}/{115}. The grains on either side of this boundary were so small that selected-area diffraction could not be used to confirm the relationship between the grains. However, the Fourier transform obtained from this lattice image (one step of the image-processing procedure) does provide this information, as illustrated in Fig.3b. The measured rotation angle between two grains ([110] rotation axis) is approximately 38.9° , as expected for the $\Sigma=9$ twin boundary. The detailed contrast of the two coherent twin boundaries indicates that the channel corresponds to bright spots; i.e., the mirror plane consists of bright spots. The atomic configuration of this boundary was determined using this information. A processed image of a (111)/(115), $\Sigma=9$ /[110] boundary is illustrated in Fig.3c and a model of the atomic configuration for this boundary is suggested in Fig.3d. It illustrates one unit of the atomic structure which includes two anti-site bonds across the boundary; the boundary structure consists of 6-, 7- and 5- membered rings.

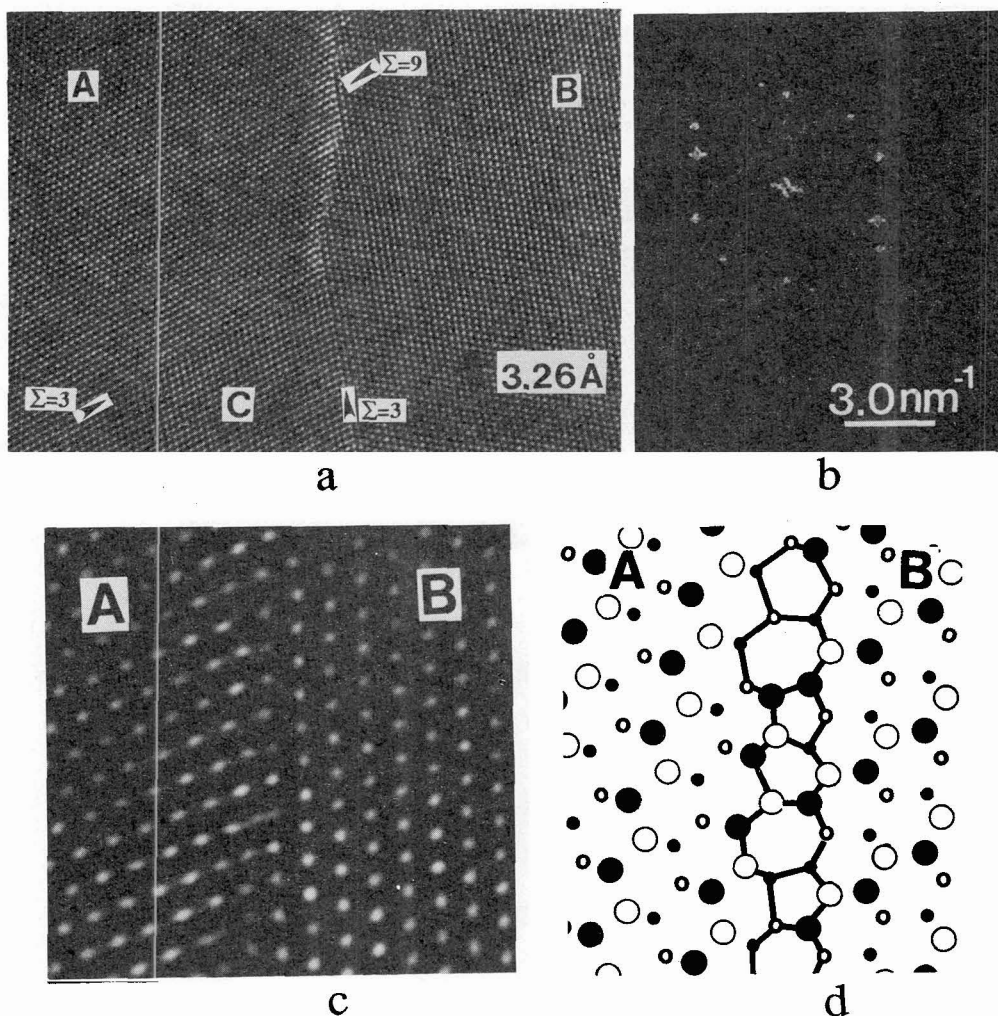


Fig. 3. A $\Sigma=9$ tilt grain boundary. a) A high-resolution image of a $\Sigma=9$ twin boundary where two coherent $\Sigma=3$ twin boundaries combine to produce a $\Sigma=9$ boundary which is faceted on the atomic scale b) A diffraction pattern produced by image processing; c) A processed high-resolution image of the $\Sigma=9$, (111)/(115), (110) tilt boundary; d) An atomic model for this boundary.

2.1 Antiphase Boundaries

An APB can be seen in Fig.4 to interact with a lateral twin boundary and a second-order twin boundary. The interaction of APBs with coherent first-order twin boundaries appears to be minimal. While the bonds across a coherent twin boundary are the same as would be found in the perfect crystal, a certain number of the bonds across both the lateral first-order twin boundary and the second-order twin boundary are, almost certainly, anti-site bonds. The APB may then interact with those interfaces without significantly changing the number of anti-site bonds. However, since an APB may itself have a local displacement field, there may be a strong reaction. An APB may therefore tend to lie parallel to either the lateral twin boundary or a second-order twin boundary.

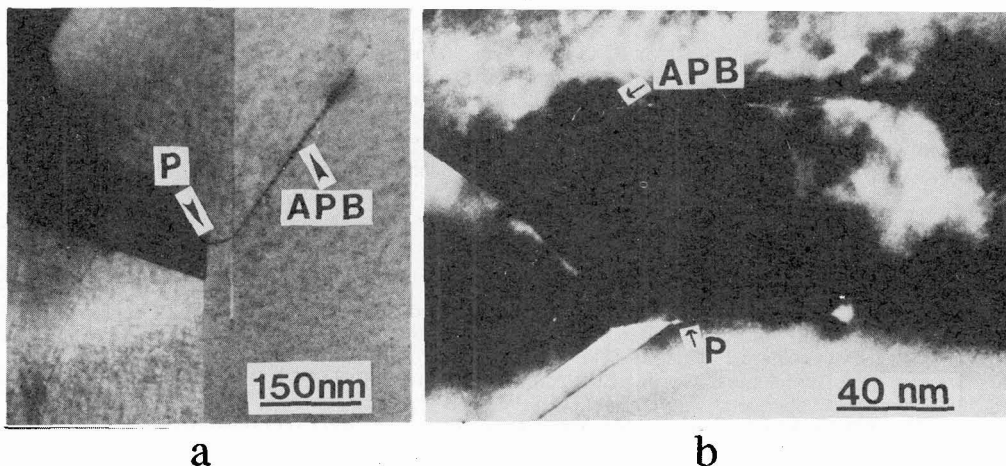


Fig. 4 Interaction of an APB with twin boundaries. a) An APB interacting with a lateral first-order twin boundary at P; b) An APB interacting with a second-order twin boundary at P.

2.2. Interaction of an APB with dislocations

Dislocations are generated in the GaAs epilayer when GaAs is grown on a (001) Ge substrate, even though the lattice mismatch is small. Dislocations are also observed to propagate through the GaAs epilayers and to interact strongly with APBs. An image recorded from a flat-on TEM sample is shown in Fig.5. The APB is visible due to the associated stacking-fault-like fringes [19]. Dislocations are present in the APB plane and run between the top and bottom surfaces of the sample. Part of a strain associated with a dislocation core is expected to be relaxed by this interaction because of the lattice translation at the APB [20].

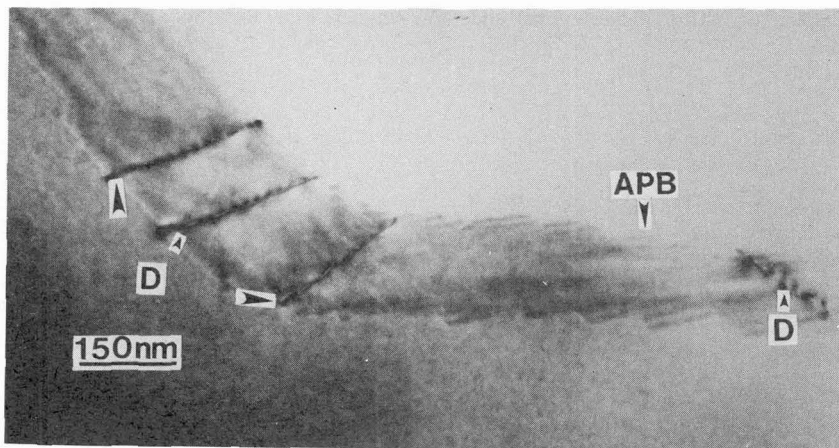


Fig. 5 Interaction of an APB with dislocations (D) in a (220) bright-field image of an APB from a flat-on TEM specimen.

SUMMARY

In order to study grain boundary structures in GaAs systematically, specific boundaries have been produced. In this paper, experimental analyses of the atomic arrangement of a $\Sigma=3$ coherent twin boundary, a (112)/(112) lateral twin boundary, and a (115)/(111) second-order twin boundary in GaAs have been illustrated, for the first time, taking account of both the polarity determination and high-resolution imaging; models are suggested which are consistent with the observed boundary structures. Interactions of APBs with grain boundaries, particularly with the lateral first-order twin boundaries and a second-order twin boundary, have been examined experimentally. The apparent strong interaction of APBs with dislocations causes the dislocations to lie parallel to the boundary plane.

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