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Atomic structure of twins in GaAs

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Two types of twins with different atomic structure may exist in GaAs: rotation type and reflection type. A selective chemical etching technique was employed to clarify which of these two twin types occurs in practical GaAs crystals. Twins in an As-rich horizontal Bridgman (HB) GaAs, a Ga-rich HB GaAs, and a liquid-encapsulated Czochralski GaAs were studied, and the results showed that all of the studied twins were rotation type. This suggests that the bonding configuration at the twin plane is a more important factor than stoichiometry of the crystal, in determining the type of twins in GaAs.

Twins are planar defects commonly observed in as-grown GaAs, which often cause serious problems to crystal growers. Several reasons were proposed of twin formation during crystal growth, including nonstoichiometry (especially excess Ga), impurities and solid particles at the solid/liquid interface, mechanical shock, sticking effect of crucibles, and rapidly diverging crystal surfaces.[1–3] These problems have been mostly solved practically, as a result of continuous efforts[3,4] to obtain good quality crystals. There are remaining questions, however, concerning formation and atomic structure of twins in GaAs.

GaAs has the zinc blende (ZnS) structure in which As (111) and Ga (111) planes are stacked alternatively following the *fcc* stacking sequence.[5] As a result, twins in GaAs may have one of two possible atomic structures shown in Fig. 1.[6,7] In the "rotation" type, positions of atoms in the twinned part of the crystal are related to the matrix atoms by the 180° rotation about the [111] twin normal direction [Fig. 1(a)] and, in the "reflection" type, by a mirror reflection with respect to the (111) twin plane [Fig. 1(b)]. These were also denoted by Holt[6] as an upright 250.53° twin and an inversion 70.53° twin. Anticlockwise rotation about $[1\bar{1}0]$ of the matrix (projection axis of Fig. 1) over 250.53° and 70.53° yields the first and second type, respectively.

Few studies[8] have been published to determine which type(s) of twins would be formed in practical GaAs crystals, and the question is still open. As indicated in Fig. 1, either Ga—Ga or As–As bonds, which usually require high formation energy, occur at the habit plane of the reflection twin whereas Ga—As bonds are preserved at the rotation twin plane. Therefore, the second type is preferred as far as the bonding energy at the twin plane is concerned. It is well known, however, that the twinning possibility during crystal growth is strongly affected by the stoichiometry of the melt. Ga-rich melts, in general, cause twins more easily,[1,4] leading to suspicion that the first type twins may also be formed in GaAs (especially in Ga-rich crystals) since these twins can accommodate nonstoichiometry related point defects by creating a Ga or As excess layer at the twin plane. It is the purpose of this letter to clarify this point, namely which type(s) of twins occur in practical GaAs crystals.

Three different as-grown GaAs crystals were studied, an undoped horizontal Bridgman (HB) GaAs, with excess As concentration (As-rich), an undoped Ga-rich HB crystal, and a Zn-doped liquid-encapsulated Czochralski (LEC) GaAs. Ga-rich HB and LEC crystals were partly polycrystalline and twins were mostly observed in the polycrystal region. For chemical etching, samples were cut to plates containing a twin at the center, so that the top and bottom faces of the plates were (111) planes parallel to the twin plane. The top and bottom faces of the plates were then lapped, mechanically polished with Al_2O_3 powders, chemically polished with $3H_2SO_4{:}1H_2O_2{:}1H_2O$ solution, and etched with $2HF{:}1H_2O_2{:}1H_2O$ solution. Etched samples were observed with an optical Nomarski microscope.

The $2HF{:}1H_2O_2{:}1H_2O$ solution used in this study attacks As (111) planes but not Ga (111) planes. In Fig. 1, it can be seen that As (111) planes are directing toward the surface from the twin plane in one part of the crystal

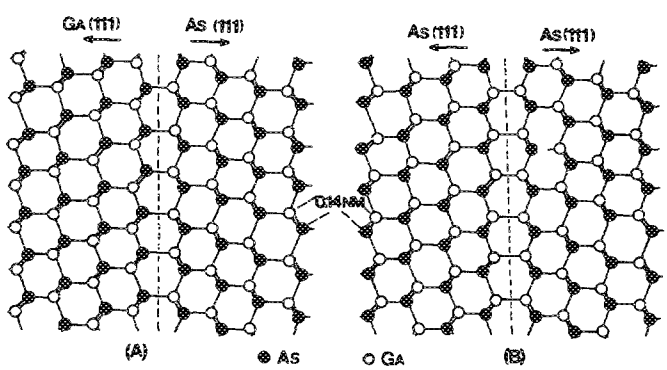

FIG. 1. Two possible atomic structures of twins in GaAs projected along $[1\bar{1}0]$ direction: (a) rotation twin formed by a 180° rotation of atoms about the [111] twin normal direction and (b) reflection twin formed by a mirror reflection of atoms with respect to the (111) twin plane.

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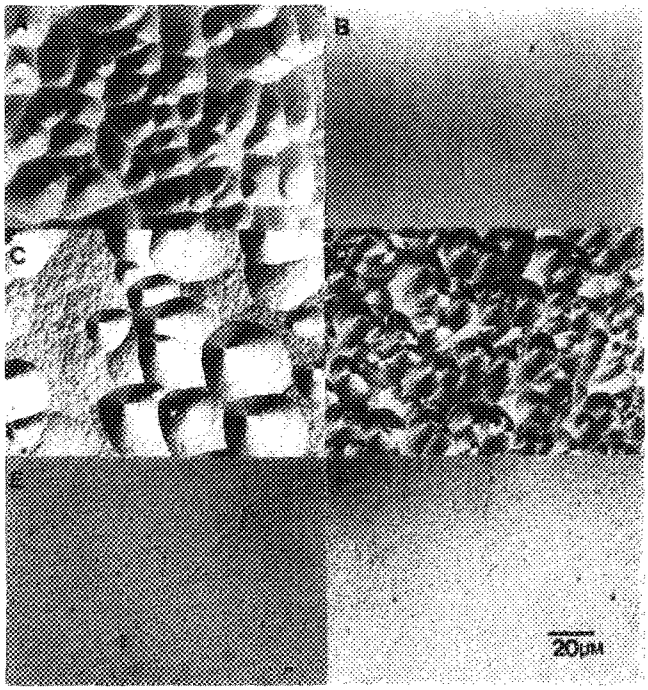

FIG. 2. Nomarski micrographs of top and bottom faces of sample plates etched with $2HF:1H_2O_2:1H_2O$ solution: (a), (b) a Zn-doped LEC GaAs, (c), (e) an As-rich HB GaAs and (d), (f) a Ga-rich HB GaAs.

and Ga (111) planes are in the other part in the case of the rotation twin, but either As (111) planes or Ga (111) planes are directing outward in both parts of the reflection twin. Therefore, the top and bottom faces of sample plates containing a twin at the center—the (111) faces directing outward from the twin plane—will be the same kind of (111) planes [either As (111) or Ga (111)] in the case of reflection type and a different kind in the case of rotation twin. This means that reactions to the etching solution must be different between the two faces if the twin incorperated at the center is the rotation type and the same if it is the reflection type.

Figure 2 is the result of the Nomarski observation of etched surfaces. It is clear that, for all the samples studied, only either one of the top or bottom faces shows etch pits (*a,c,d*) but the other face does not show any etch pit (*b,e,f*). Hence, the two faces show different reaction to the etching solution from each other, proving that all the observed twins are rotation type regardless of the stoichiometry of the crystal and the technique employed to grow the crystal. The triangular shape of the etch pits shows that the etched planes are (111) planes. It can also be seen by counting the number of etch pits that the Ga-rich HB GaAs and LEC GaAs have a higher density of dislocations than As-rich HB GaAs.

As was discussed before, the rotation twins are preferred in terms of bonding energy at the twin plane but the reflection twins have advantages in accommodating nonstoichiometry. From our result, it is concluded that the bonding configuration at the twin plane is a more important factor than the stoichiometry of crystal in determining the type of twins in GaAs.

Computer simulation of high-resolution transmission electron microscope (HRTEM) images of twins in GaAs was also performed in this study, using the CEMPAS program.[9] It was attempted by previous investigators[8] to employ the HRTEM technique to determine twin structure in GaAs, since this technique, in principle, is able to image positions of atoms directly and gives fine details of atomic structure as well. The results of simulation study in this work, however, showed that it will be difficult to reveal detailed atomic structure and thereby determine the type of twins in GaAs using the HRTEM technique, even with advanced instruments available at the present time. Further details of the simulation results will be published elsewhere.

In summary, atomic structure of twins in an As-rich HB GaAs crystal, a Ga-rich HB GaAs, and a LEC crystal was studied by a selective chemical etching technique. It was concluded as a result that all the studied twins were rotation type formed by a 180° rotation of atoms about the [111] twin normal direction. This suggests that the bonding configuration at the twin plane is the critical factor in determining the type of twins.

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