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Transmission electron microscopy observations of antiphase boundaries in CdTe

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Specimens from CdTe crystals, prepared by two different methods were examined by transmission electron microscopy. Antiphase boundaries were observed in both the {110} and {311} planes. Comparatively regularly ordered partial dislocations with a Burgers vector $b = a/6\ \langle 112 \rangle$ were found in both cases. The distance between partial dislocations is about 6–8 nm. The probable formation mechanism of these boundaries is discussed.

1. Introduction

Cadmium telluride (CdTe) crystallizes in the cubic sphalerite (zinc blende) type structure with space group F $\bar{4}$32 and is susceptible to twining. The relations between the host matrix and the twinned one can be described in several different ways, as is discussed by Durose and Russell [1]. The sphalerite structure can be described as two face centred cubic (f.c.c.) lattices displaced by an $a/4\langle 111 \rangle$ vector. The metal atoms occupy the first f.c.c. lattice and the non-metal atoms the other one. The antiphase boundaries (APB), which are the boundaries that cause a change in the polarity of the $\langle 111 \rangle$ direction in sphalerite type structures are described theoretically by Holt [2]. Two basic types of APBs have been distinguished by the author. The first type (I) is described as a plane containing $a/4\langle 111 \rangle + L$ vectors (where L is any f.c.c. vector) and therefore contains atom positions of both f.c.c. lattices. The second type (II) APB does not contain a $a/4\ \langle 111 \rangle$ vector and therefore has atom positions of only one f.c.c. lattice (the {111} APB). Two sub-types are distinguished in type I: type I(i) containing only one $a/4\ \langle 111 \rangle$ vector (the {311} APB) and type I(ii) an APB which contains two $a/4\ \langle 111 \rangle$ vectors and in this way fully determines the APB's plane as {110}. It should be pointed out that type II APBs contain either A–A or B–B* "wrong" bonds only, the type I APBs have both A–A and B–B ones. These boundaries can also be described as boundaries formed by twisting around a crystallographic axis [3].

The use of many different methods for the characterization of the grain boundaries in CdTe are described in the literature with etching and consequent examination by optical or scanning electron microscopy being the most frequently used techniques [4–7]. However no detailed information on the boundary structure can be obtained by this technique. The defects discussed previously are structural and transmission electron microscopy (TEM) images are required to gain information on them. However difficulties exist in the TEM specimen preparation processes. In recent works [8–10] TEM images of the $\Sigma 3$ and $\Sigma 25$ boundaries, as well as high resolution images of extrinsic and intrinsic stacking-faults due to the dissociation of a 60°-edge (with a Burgers vector $b = a/2\ \langle 110 \rangle$) have been reported. The results of TEM observations of APB boundaries in CdTe crystals are presented in this paper.

2. Experimental procedure

CdTe crystals grown by the Bridgman method from nearly stoichiometric melts were used for the examination. Specimens were prepared either by the "suspension" method (wet grinding in pure ethanol, consequent deposition of the suspension on the perforated carbon foil and careful drying) or by local chemico–mechanical thinning with 2.5% bromine in a methanol solution [8]. The first method is not to be recommended for the evaluation of the structural quality of CdTe, due to the possible introduction of many defects in the preparation processes. If the purpose of the experiment is the investigation of macrostructural defects, then it is believed that this method is useful.

The investigations were carried out on a Philips-420 transmission electron microscope operating at a 120 kV accelerating voltage. The orientation of the specimens were determined in selected area electron diffraction mode and the dislocations were observed in diffraction contrast mode.

3. Experimental results

The diffraction pattern shown in Fig. 1b, shows that the images on Fig. 1 (a and c) and Fig. 3 (a and b) are

*We will denote A as the low valence atom (Cd) and B as the higher valence Te-atom.

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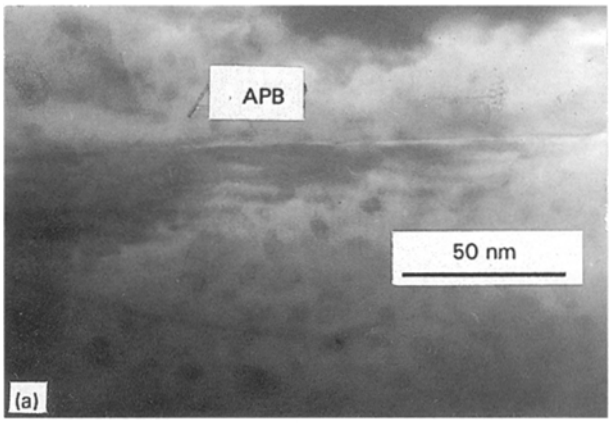
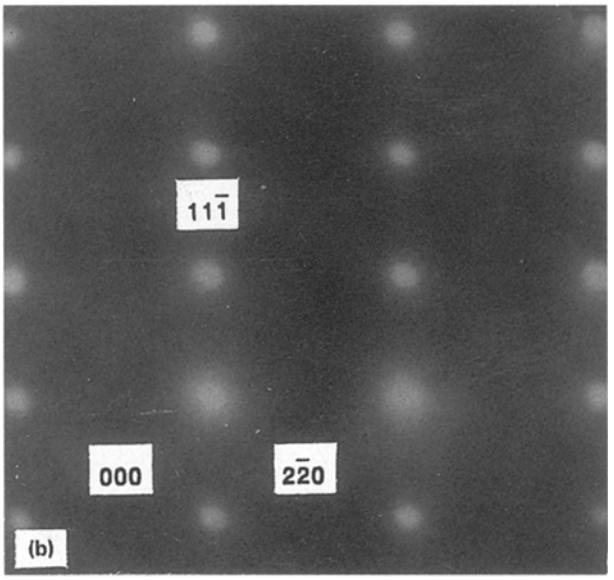




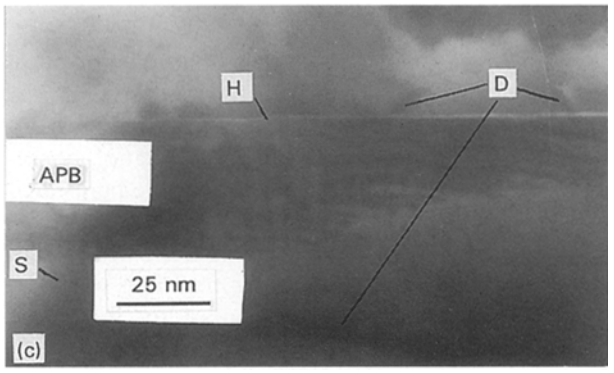


Figure 1 (a) Bright-field image of a {110} APB. The marker represents 50 nm. (b) Corresponding to Fig. 1a diffraction patterns (c) The two beams, (000) and (11$\bar{1}$) reflections, TEM image of {110} APB.

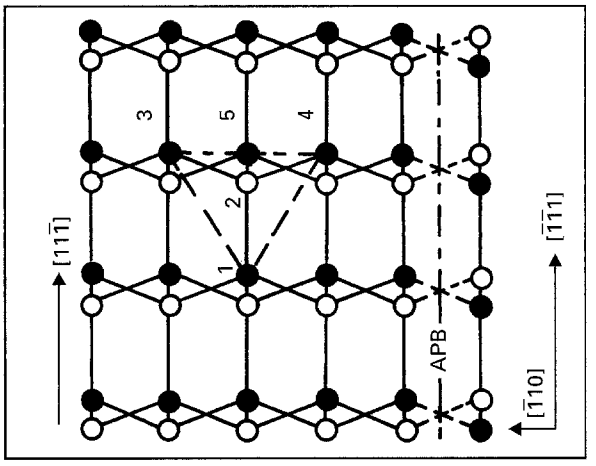
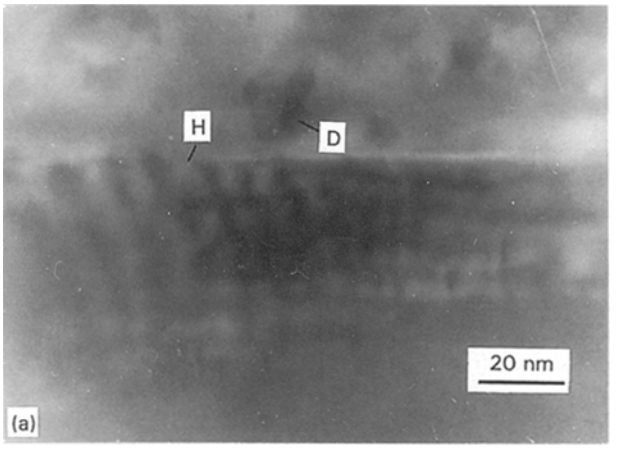


Figure 2 Projection of (112) section of CdTe lattice. 1–3–4 projection of 4Cd + 1Te tetrahedron. If atom (1) and atom (2) lie in the projection plane, atoms 3 and 4 are at 1/6⟨112⟩ distance above and the atom 5 is at 1/3⟨112⟩ under the projection plane. The APB is perpendicular to the sheet and intersects it in the APB line.



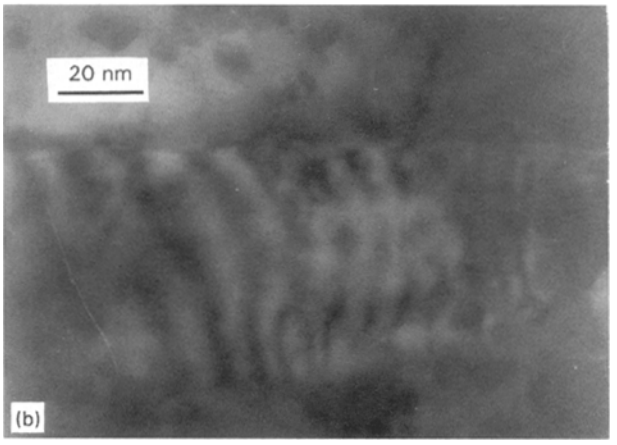
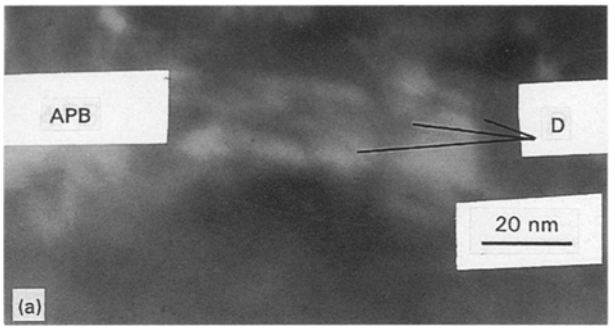
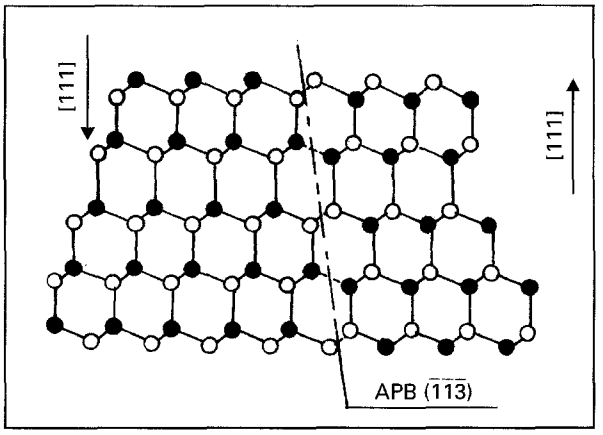


Figure 3 (a) Bright-field, two beams- (000) and (11$\bar{1}$), image of {110} APB (b) Dark-field image, reflection (2$\bar{2}$0) image of the same APB.

formed along the ⟨112⟩ zone axis. Since neither "spot splitting" nor reflections from a second crystal lattice were observed it may be concluded that the boundary (marked with APB on Fig. 1c) is type I(ii) an antiphase APB lying in the {110} plane. A model of such a boundary is shown in Fig. 2a. Relatively well ordered dislocations, spaced at about 6–8 nm separations can be seen on the bright-field images area H in Fig. 1 (a and c) and Fig. 3a, of the {110} APB. They form a honeycomb network. A part of the dislocations are out of contrast on Fig. 3b and it could be suggested that their Burgers vectors are either $b = a/6[\bar{1}12]$, $b = a/6[\bar{1}1\bar{2}]$, $b = a/6[1\bar{1}0]$ or the opposite ones.

The analagous image which is Fig. 4 was observed from a specimen prepared by chemico–mechanical thinning [8]. The APB lies in the {311} plane and its





(b)

Figure 4 (a) Dark-field image reflection (111) image of a {311} APB. (b) Projection of {110} section of the CdTe lattice. The APB is perpendicular to the sheet and intersects it in the APB marked line.

model in the {110} projection is described by Holt [2]. Dislocations form a network and are spaced at distances of about 6–8 nm. The structure of this network can be envisaged as consisting of distorted parallelograms. Such a configuration will be unstable [3] and the real network probably has a honeycomb structure. More precise investigations of this boundary were complicated due to the sample thickness and the tilt position of the APB in the specimen.

4. Discussion

There are several possible theoretical explanations for the presence of APBs in the crystals.

(1) Splitting of a 60°-edge (so called twinning) or the splitting of a screw dislocation into two partial ones may cause APB type II [2].

(2) Stacking-faults created by the growth conditions near the solid–liquid interface during the crystal growth and forming a closed contour might be bordered by APBs. No dislocations due to the APB are expected in the boundary plane provided that the electrostatic interaction between atoms on both sides of the APB is neglected.

(3) The APB could be the result of a plastic deformation and this is the probable cause of the observation of dislocation networks in this case.

As the observed dislocation networks (particularly those of Fig. 1c and Fig. 3 (a and b) have changed their "honeycomb" dimensions as well as coming out of contrast in different parts of the network it could be concluded that the APB observed is a general twist boundary [3]. This boundary is characterized by non-perfect coincidence of the twist axis and the crystallographic axis of the lattice (in this case the [1$\bar{1}$0] axis) while the Burgers vectors and the lines of the forming dislocations are exactly fixed. That is why the dislocation network does not lie exactly in the boundary plane. The presence of a minimum of three independent series of dislocations is required in this case [3]. The intersection of external dislocations (marked by D on Fig. 1c and Fig. 3a and a stacking fault (marked by S on the same figures) have additionally complicated the discussed case. The Burgers vectors and the lines of the initial dislocations are not known and we can only speculate on the characteristics of the dislocation network. A final conclusion as to whether a prismatic glide [11] or a normal glide in the corresponding glide planes [12] caused the observed defects cannot be provided for this reason.

5. Conclusion

The real situation in this material is more complicated than any ideal case but it may be concluded that deformation stress is the most probable reason for the formation of APB in the cases under discussion.

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