TEM observation of two- dimensional defects in CdTe crystals

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A specimen from a melt-grown CdTe crystal was prepared by the “suspension” method. Selected area electron diffraction (SAED) image revealed the presence of stacking faults and a twice twinned crystal lattice in the examined specimen. Many dislocations, stacking faults as well as first-order and second-order twin boundaries, accompanied by many dislocations lying in (or close to) the grain boundary plane were observed in the diffraction contrast mode images. The main types of the existing defects were modeled, and the corresponding SAED pattern images were successfully simulated.

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1. Introduction

Cadmium telluride (CdTe) is a II-VI binary compound that crystallizes in a sphalerite type lattice. CdTe crystals are usually grown by the Bridgman method in evacuated and sealed quartz ampoules from melts. Nevertheless, independently of the growth method, the crystals have two- dimensional defects- mainly twins and stacking faults. However, the main applications of this material (X- and γ- ray detectors, infrared optics etc.) require high quality crystals. This is why it is very important to characterize the main defects and their natures in order to avoid their formation.

There are few published results of transmission electron microscopy (TEM) studies of twin and sub-grain boundaries in CdTe crystals [1- 5], as it is very difficult to prepare specimens by a simple technique. Earlier, we reported in brief [5] results of the use of the so-called “suspension” method, and deduced that some stacking faults were probably introduced during the sample preparation. Here, we report results of a TEM observation of a CdTe specimen prepared by the suspension method, and a detailed characterization of the observed defects.

2. Theory

The crystal lattice of compounds with a sphalerite type structure, consists of two interpenetrating face-centered cubic (f.c.c.) sub- lattices of low- and high-valence atoms, respectively. The sub-lattices are displaced from one another by one quarter of the unit-cell volume diagonal- $a_o/4$ <111> (a_o- lattice parameter). The structure can be described as three double atomic layers (of low- and high-valence atoms), consequently ordered at $a_o/3$ <111> along the <111> direction. The low- and high-valence atoms, have identical coordinates and are displaced perpendicularly by $a_o/4$ <111> in the double atomic layers. Then, the atomic stacking along <111> direction can be represented as …γCαAβBγCαAβBγC… where the layers of low-valence atoms are designated by small Greek letters and the layers of high-valence atoms are designated by capital Latin letters- Fig. 1a). The absence of a center of symmetry makes the <111> direction (as well as some other directions, e.g. <112>, <001> etc.) polar. This fact is reflected in two ways: firstly, the atomic layers’ order in the positive and negative directions of the polar directions is different, and secondly, there are two different gliding planes between the low- and high- valence atomic layers: one lying in the double atomic layers and another between these layers. The individual changes in the order of the double atomic layers are determined as stacking faults: intrinsic (when a double layer is missing- for example: …γCαAβBγCαA_γCαAβBγC… where **”_”** marks the position of the missing double βB-layer- see Fig. 1a), or extrinsic (when a double layer is added- for example: …γCαAβBγCαAβB γCαAβBγC…- where the added double βB- layer is underlined).

The twins in the zone axis <011> in compounds with diamond or sphalerite type lattices could be described in several ways, but here we will prefer the one discussed in [6]- as a tilt at θ = 250.53° and at Θ = 109.47° about <011> for first-order twins.

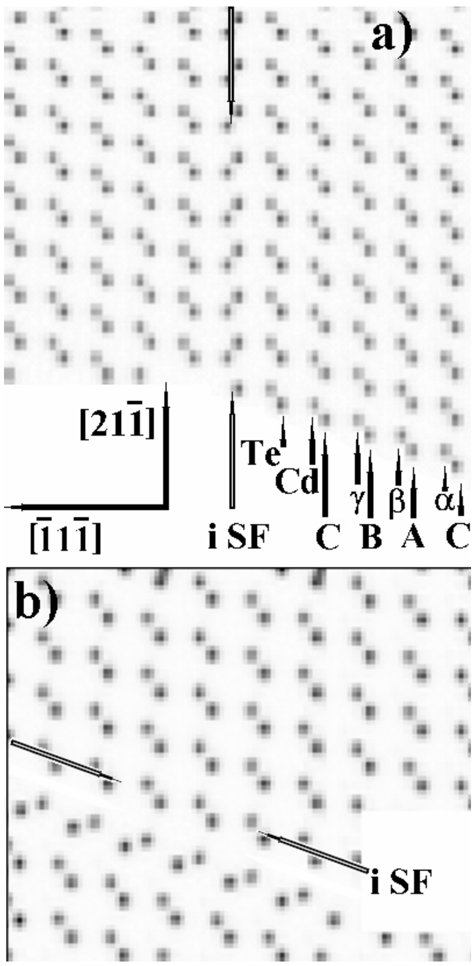

Fig. 1. a) Part of the supercell (viewed along [011]) containing an intrinsic stacking fault (the position of the missing atomic layer is marked by arrows). The Cd-atomic layers are marked by Greek letters and the Te-layers by capital Latin letters. b) Part of the supercell (viewed along [011]) containing an intrinsic stacking fault (the position of the missing atomic layer is marked by arrows).

3. Experimental

A crystal piece was cleaved along {011} from a melt-grown CdTe crystal, from an area that included three grains. The specimen for TEM observation was prepared by the so-called "suspension" method (grinding a small piece of the crystal in an agate mortar in pure ethanol and deposition of the fine suspension on a perforated carbon foil). The observation was carried out in a PHILIPS-420 TEM microscope at 120 kV accelerating voltage.

4. Results and discussion

There are only a few CdTe flake-like particles deposited on the carbon foil, with appropriate thickness for the TEM study. We obtained a bright field (BF) diffraction contrast TEM image and a selected area electron diffraction (SAED) patterns' image in the [011] zone axis, from an area that contained two- dimensional defects- Figs. 2) and 3) from only one crystal particle.

The SAED pattern- Figs. 2a) and 4a) from the entire area of the specimen revealed the presence of a doubly-twinned lattice (tilted at θ = 250.53°- marked by T_2 in Fig. 2a) and at Θ = 109.47° about [011]- marked by T_3 in Fig. 2a). Some additional patterns denoted by D'=D" and D_1= D_2- Fig. 4a) that correspond to 5/6 $d_{(222)}$= 0.225 nm and to 3 $d_{(224)}$= 0.397 nm can be observed in the SAED pattern- Fig. 4a), and could be related to secondary effects of superposition of the twinned and the host lattices along the zone axis [3]. The reflections of the host lattice are split and strongly elongated. The basic reflections of the host lattice form a network with basic reflections $d_{(111)}$= 0.3741 nm marked by black circles in Figs. 2a) and 4a). There is also an outer network (marked by a black rhombus in Fig. 4d)) determined by the strongly elongated patterns that coalesce into lines. This network, which corresponds to reflections due to an interplanar distance 8.33% smaller than $d_{\_(111)}$= 0.3472 nm, is also observed in the SAED pattern- Figs.2a) and 4a).

The diffraction contrast image- Figs. 2b), 2c) and 3), can be divided conditionally into three main parts, according to the defects observed in different parts of the specimen:

The first one is situated around the central part of the specimen and is strained and occupied by dislocations (some of them marked by D in Fig. 2b)) with lines probably slantingly intersecting (011) and separate stacking faults (SF), some of them marked by SF in Fig. 2b).

The second one is occupied by SF lying in {111}, i.e. in planes declined at 30° with reference to the plane of the specimen- Fig. 2c). These SF, as well as the dislocations and SF described in the previous item, are probably caused by the mechanical stress during the specimen' preparation process. The probable mechanism for this is described in [5]: 60°- dislocations, e.g. with a Burgers vector **b**=1/2<011>, and lines along <011> are introduced into the crystal lattice. These dislocations dissociate into stacking faults bordered by partial 30°- and 90°-dislocations with **b**=1/6 <112> probably from the so-called gliding set [7].

The third one is situated between the boundaries marked by A,B,C,E and F in Fig. 2 b). This area is occupied by the first-order twins revealed in the SAED images in Figs.2a) and 4a). The lattice between the boundaries EFCE' is probably tilted at Θ= 109.47° about [011]- reflections from this lattice are designated as T_3- see Fig. 2a), while the lattice between the boundaries ABCE' is probably tilted at θ= 250.53°- reflections are designated as T_2 in Fig. 2a). The corresponding first-order twin boundaries (between the host and twinned lattices) and second-order twin boundaries (between the twinned lattices) were not exactly determined, e.g., by analysis of stereo pairs, as only a few of them were parallel to the zone axis. Nevertheless, the CF-boundary (Figs. 2b) and 3)) could be determined as the {111}-{111} boundary; the ABA'B' and BCC'B' boundaries are declined with reference to the zone axis and the A'B'CE' boundary is

{011}-{114}, i.e. perpendicular to the zone axis. Irregular dislocation' networks (marked by D_T in Fig. 3)) could be observed in every declined boundary.

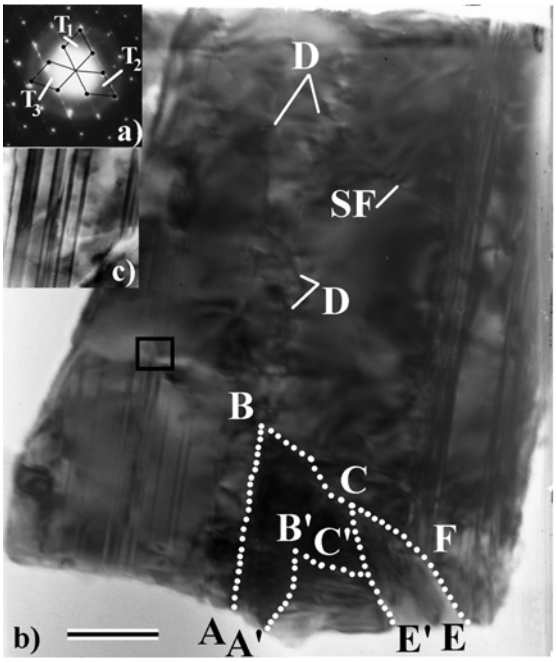

Fig. 2. a) The SAED pattern- obtained along the [011] zone axis. T_1 marks the basic reflections of the host lattice, T_3 the basic reflections of the lattice tilted at Θ= 109.47°, and T_2 the basic reflections of the lattice tilted at θ= 250.53°. b) The corresponding TEM image. The marker represents 1 μm. c) A five-times magnified image of the stacking faults in the area marked by the black rectangle in Fig. 2b).

The SAED pattern simulations- Figs. 4b), c) and d), were performed by the software package MSLICE [8]. Parts of the supercell used for simulation of the SAED pattern of intrinsic stacking faults is shown in Figs. 1a) and b) and has dimensions of about 10x10x40 nm. The corresponding SAED pattern is shown in Figs. 3c) and in the upper part of Fig. 4d). The observed change of the distance between the basic reflexes of the two pattern networks (the first one determined by the $d_{(111)}$ reflections- black circles and the second by the elongated reflections- the white rhombus in Fig. 4d)) amounts to 8.33%, which coincides with the experimental findings- Figs. 2a) and 4a).

The super-cell used for simulation of the first order twins is described in more detail in [3], and the corresponding SAED pattern is shown in Fig. 4c). The experimentally observed reflections D'=D" and D_1= D_2 in Fig. 4a) are successfully simulated- Fig. 4c), and are probably due to a superposition of the host and the twinned lattices along the zone axis as they correspond to the reflections marked by the same D_1, D_2 and D' in the simulated image- Fig. 4c).

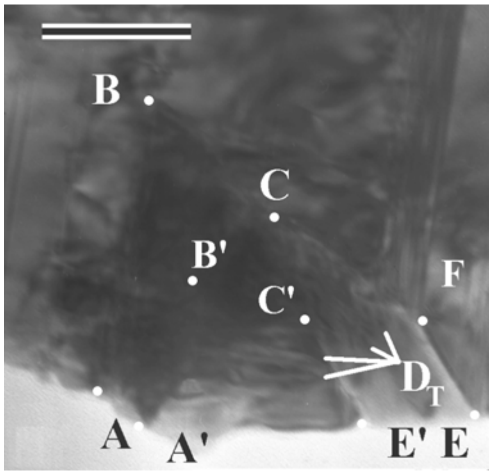

Fig. 3. A magnified part of the BF image shown in Fig. 2b).

5. Conclusions

A specimen for TEM examination was prepared by the suspension method from a melt grown CdTe crystal. Many intrinsic stacking faults and dislocations were observed in the specimen. We argue that they are probably caused during the specimen preparation. It may be concluded that the observed first-order twins (tilted at Θ = 109.47° and at θ = 250.53° about [011]) can not be related to the specimen preparation process. The observed dislocations in every twin boundary, declined with reference to the zone axis, can also not be considered as introduced into the crystal during the treatment of the specimen.

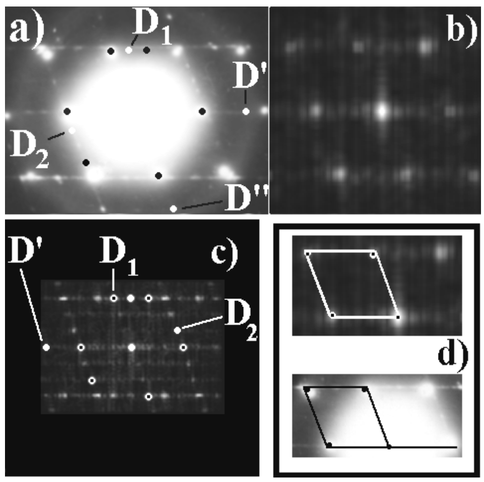

Fig. 4. a) The SAED pattern from Fig.2a). The black dots denote reflexes that are equal to $d_{(111)}$= 0.3472 nm.b) A simulated SAED pattern deduced from the supercell containing intrinsic SF and shown in Figs.1a) and b). c) A simulated SAED pattern deduced from the supercell presented in [5]. D_1=D_2 and D" mark reflections that correspond to the D_1= D_2 and D'= D" reflections from the experimentally obtained image in Figs. 2a) and 4a). d) Separated parts from Figs. 4 a)-lower image and b)- upper one.

Acknowledgements

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