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Transmission electron microscopy characterization of the deformation of CdZnTe single crystals induced by nanoscratching

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The deformation characteristics of soft-brittle CdZnTe single crystals induced by nanoscratching were investigated using cross-sectional transmission electron microscopy. Significant pile-up was observed, but no amorphization phases existed. Twins, stacking faults and nanocrystals were found in the scratched subsurface. This is somewhat different from the deformation patterns obtained from our previous nanogrinding study, where twins were seldom observed. The deformation mechanisms were discussed.

Keywords: Compound semiconductor; Nanoscratching; Deformation; Transmission electron microscopy (TEM)

As a II/VI compound semiconductor, cadmium zinc telluride (CdZnTe or CZT) single crystals have received extensive attention due to their unique properties, such as high electro-optic coefficient, transparency in the mid-infrared region, high electrical resistivity and relatively good charge transport properties [1,2]. CZT is now widely used in applications like radiation detectors, photorefractive gratings, electro-optic modulators, solar cells, and terahertz generation and detection [2]. CZT single crystals with specific stoichiometries, e.g. $Cd_{0.96}Zn_{0.04}Te$, are often used as substrates to grow epitaxial mercury cadmium telluride (MCT) for the manufacture of infrared detector arrays due to their perfect lattice matching [3,4], as well as excellent thermal expansion and valence compatibility [5]. In most of these applications, CZT must be machined from an as-grown ingot into a wafer form with stringent requirements on surface integrity [2]. This is because any surface and subsurface damages induced by the machining can significantly affect the mechanical and electrical properties of semiconductor materials, and consequently the performance of CZT-based devices [6–8].

Grinding is an essential process for machining CZT wafers [9–13], which involves repeated interactions of "scratching" between abrasive particles and the work material. As CZT is a unique material that peculiarly combines "softness" and "brittleness", its deformation and removal mechanisms are expected to be different from our conventional wisdom on semiconductor solids such as silicon [14,15] and gallium arsenide [16], hard and brittle materials such as tungsten carbide [17] and silicon carbide [18], or even metallic glasses [19,20]. Previous studies have indicated that a mixed mode of brittle and/or ductile removal exists in the grinding of CZT wafers [13]. Our recent transmission electron microscopy (TEM) characterizations of ground CZT subsurfaces revealed that lattice defects and nanocrystals were generated by the nanogrinding process [9]. Nevertheless, until now, little has been done to increase the fundamental understanding of the grinding-induced deformation of this material class, and the effect of mechanical loading/unloading conditions on the material removal remains unclear [9–13]. As grinding is a complicated machining process that involves numerous repeated and severe interactions between diamond grits and the work material, it is thus impossible to isolate the effect of mechanical loading on the material deformation and removal. Nanoscratching mimics the processes involved in an individual grit-work interaction event in a controlled manner [16,21,22], and thus allows the systematic understanding the effect of the grinding-induced loading/unloading on the surface and subsurface damage caused by grinding.

In this study, we investigate the deformation nature of CZT single crystals induced by nanoscratching using cross-sectional TEM. Using the TEM characterization

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of nanoscratch-induced deformation of CZT, detailed here for the first time, significantly different deformation mechanisms in the CZT single crystals are identified and the underlying fundamental reasons are discussed.

The nanoscratch experiments were performed on as-received $Cd_{0.96}Zn_{0.04}Te$ (1 1 1) wafers in a Hysitron Triboindenter®, where a Berkovich tip with a tip radius of 100 nm was used. The reason we chose the Berkovich tip is that it has a three-sided face and an included angle of 142.3°, which is closer than a conical tip to the geometry of diamond grits used in grinding. The scratches were made along one of the CZT ⟨1 1 0⟩ directions on the CZT (1 1 1) surface. Although CZT is a crystal with polarity, the effect of polarity on the mechanical properties is insignificant [5], especially when the deformation is on the micrometer scale. The normal load was kept at a constant 1 mN during the scratching. Due to the brittle nature of the CZT crystals, the cross-sectional TEM specimens were prepared using a modified tripod method [23], where a long scratch (of ~500 μm) was made using a high load transducer attached to the indenter. The ⟨1 1 0⟩ cross-sectional TEM specimen of the scratch was prepared by cutting and grinding, followed by ion beam thinning using a precision ion polishing system (Gatan Inc., USA) with an Ar ion beam at an energy of 3.5 keV. It should be noted that the TEM specimens were prepared in such a way that the electron beam is parallel to the scratch directions to avoid any possible damage. TEM investigations were carried out on a Philips Tecnai F20 transmission electron microscope operating at 200 kV.

Figure 1a is a cross-sectional on-zone bright-field (BF) TEM image of the scratch made at a normal load of 1 mN, showing a triangle-shaped impression. The depth of the residual impression is ~200 nm, causing a damaged layer ~3 μm in depth. Figure 1b shows an enlarged image of the damaged region, so that the severe deformation can be seen clearly. A relatively light contrast is seen directly beneath the scratch, indicating that the crystal orientation in this region is different from the original CZT ⟨1 1 0⟩ direction.

Figure 1c and d shows two selected area electron diffraction (SAED) patterns acquired from different locations of the scratch impression, as indicated by the white and black circles in Figure 1b, respectively. The SAED pattern shown in Figure 1c was acquired from the area next to the shoulder of the scratch. A set of diffraction spots, indicated by the solid white arrows, was superimposed on the CZT ⟨1 1 0⟩ diffraction pattern and identified as the diffraction spots from the twin structures. The streaks along the normal direction of {1 1 1} are attributed to the high density of {1 1 1} planar defects. Twins were also found to be formed at the shoulder of the scratch impression in GaAs [16], whereas no twin was formed at the similar location in the scratched Si [24]. Figure 1d shows an SAED pattern acquired from the slope of the scratch impression, in which the diffraction spots are elongated and more diffraction spots can be seen, suggesting that the lattices were severely deformed and nanocrystals were formed. No diffused diffraction ring could be observed, indicating that no amorphization occurred during the scratching.

Significant pile-up was observed in the scratched CZT sample, as shown in Figure 1e, which was taken from the area marked by the white square in Figure 1b. The surface of the CZT substrate prior to scratching is highlighted using the dashed line. The pile-up is clear and has a height of ~40 nm, 20% of the penetration depth. The height of the pile-up area in CZT is much greater than that in Si, which is less than 5% of the penetration depth [24]. Inside the pile-up, severely deformed lattices are seen, as confirmed by the high-resolution (HR) TEM image in Figure 1f. This suggests that, when the CZT material is squeezed during scratching, lattice defects are simultaneously induced. The propagation and accumulation of these lattice defects lead to a mass migration until finally a pile-up is formed. In other words, the formation of lattice defects "softens" the lattice, thus making it easier for a pile-up to form. In contrast, in the case of Si, there is no lattice defect in the shoulder of the scratch, so deformation of the material is thus harder [25,26]. This finding suggests that the CZT materials flow easily with the help of the formation and propagation of lattice defects, mainly twins, in contrast to Si.

Figure 2a shows a further enlarged cross-sectional TEM image of Figure 1b acquired from the scratch impression. The HRTEM image shown in Figure 2b was acquired from the region marked by the black square in Figure 2a. Nanocrystals with sizes ranging from 10 to 20 nm were observed. These nanocrystals kept the same crystal structure with the original CZT, but orientated differently. Some of the lattice planes can be determined as CZT {1 1 1} or CZT {1 1 0} planes, as marked in Figure 2b. It should be noted that the lattice could not be clearly seen in some nanocrystals in Figure 2b, because these nanocrystals were not orientated in any zone axis. Nanocrystals were also found in the CZT sample ground using an ultrafine diamond grit wheel [9]. We cannot see any amorphous phase in the scratched area from the HRTEM images in Figure 2b, which is in good agreement with the SAED analysis.

Figure 2c shows the HRTEM image of the region marked by the white square in Figure 2a. High-density stacking faults are apparent, indicating that stacking faults associated with partial dislocations are easily generated in the deformed CZT when compared with the situations in deformed Si, in which perfect dislocations were formed [26]. The fact that the stacking fault energy of CZT is in the range of 10–16 mJ m^{-2} [27], which is much lower than that for Si (69 ± 7 mJ m^{-2}) [28], suggests that stacking faults associated with partial dislocations are one of the main deformation mechanisms in semiconductor materials with low stacking fault energy.

It is of interest to note that no amorphization occurred during the scratching on CZT from both the SAED patterns and HRTEM images. II–VI compound semiconductors usually have covalent and ionic bonds coexisting in their crystal structures [5]. The mechanical properties of the binary compounds originate primarily from the weak covalent–ionic bonding of the II–VI elements. The introduction of third elements, e.g. adding Zn into a Cd–Te lattice to form the CdZnTe ternary compound, further weakens the bonding [5]. When under mechanical loading, such as nanoscratching, slip