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Quality Improvement of CdZnTe Single Crystal by Ultrasound Processing

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Abstract: **Intrinsic defects and contaminations removal from the undoped p-type $Cd_{0.96}Zn_{0.04}Te$ single crystals has been achieved by the ultrasound vibration processing at the room temperature. Surface analysis based on Auger Electron Spectroscopy, Energy Dispersive Spectroscopy, and Scanning Electron Spectroscopy shows a significant reconstruction of the crystal surface after processing, namely, the appearance of numerous "volcano craters" and triangle-shaped defects with a typical size of 0.2-5.0 µm. Elemental analysis of these defects shows that they are Te inclusions emerged on the surface. The regular crystal surface outside the defects also displays a considerable enrichment by Te. Distinct presence of copper is found in both the thin surface layer and in the defects emerged on the surface. The surface reconstruction is associated with a remarkable change in the bulk material properties, electrical (an increase in the resistivity by a factor of ~ 6) and optical (an IR transmittance increase). A post-polishing following the ultrasound processing makes the CdZnTe material more stable and reliable for a wide range of device applications.**

Keywords: B2. Semiconducting II-VI materials; B2. Semiconducting cadmium compounds; A1. Impurities; A1. Defects; A1. Purification

1. Introduction

Ultrasonic Vibration Processing (UVP) discovered in the mid 70's has become an effective instrument for defect engineering of a wide class of semiconductor materials, particularly, II-VI and III-V compounds. Non-equilibrium in its origin, UVP is one of the technological approaches that realize a *defect engineering concept* for improving the performance of semiconductor materials and devices at relatively low temperatures (see [1] and references cited in).

It is well-known that defects and their complexes in real single crystals exist in stable, unstable and metastable configurations. UVP is based on the coupling of the ultrasonic vibrations with a system of the extended defects such as dislocations, grain boundaries, inclusions and precipitates, and thereby with point defects, both of the impurity and native origin. The ultrasound mechanical vibrations can trigger the crystal defect reactions by transforming the existing bound (metastable) defects into unstable ones at relatively low temperatures (generally, below 100°C), and assist the system of crystal defects in reaching a new favorable position, which has the lowest total energy. Since the introduced power is lower than the threshold level, it does not generate new defects in material (see [1] and reference [1] cited in). Thus UVP is nondestructive technological method. As a consequence of aforesaid transforming of defect structure, the ultrasonically treated materials and devices have improved properties; they become more stable and resistant to aging and degradation.

Intuitively, the potential of UVP should be substantial in devices with a significant level of byproduct defects, or ones produced from materials having a moderate initial quality due to inherent growth defects. In both cases the use of ultrasonic processing by itself or in combination with other technological methods allows achieving the superior final quality.

Cadmium Telluride (CdTe) and Cadmium Zink Telluride (CZT) bulk crystal materials are in great demand for X-ray and gamma imaging spectroscopy [2]. Additionally, they are basic bulk materials for the fabrication of infrared detection and imaging systems [3].

The performance of CdTe single crystal and its ternary derivative CdZnTe usually suffers from a surplus content of Te atoms. This stoichiometric deviation stems from inherent features of crystal growth, namely, the retrograde solid solubility effect which is associated with a Te-rich side position of the congruent melting point of the material. During the cooling-down of an as-grown crystal the surplus Te atoms nucleate in extended precipitates of typical sizes of 10-50 nm [4, 5]. Inclusions are another possible source of surplus Te in the crystal. They are formed by capturing of melt-solution droplets from the diffusion boundary layer adjacent to the growing interface enriched by the rejected excess component (Te). Typical inclusion sizes are 1-2 µm although sizes of 30 µm and larger have been observed in material grown by the Bridgman techniques [4, 6].

It is now well understood that the deviation from stoichiometry due to Te surplus degrades the structural performance of the material by introducing stress and crystal lattice distortion which are relaxed by formation a three-dimensional dislocation network in the as-grown crystal [4]. Moreover, a post-processing treatment commonly used for the reduction of the Te excess content (high temperature annealing under the Cd-vapor atmosphere) results in the generation of an additional dislocation network [7].

The excess Te content can also deteriorate the electrical properties of the material since Te interstitials released from the cluster become the high mobility defects. Thus they are able to associate with the numerous intrinsic and impurity point defects and define in such manner the Fermi level position, i.e., the conductivity of the material [8], the

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