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Towards defect-free epitaxial CdTe and MgCdTe layers grown on InSb (001) substrates

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ABSTRACT

A series of three CdTe/$Mg_xCd_{1-x}Te$ ($x\sim0.24$) double heterostructures grown by molecular beam epitaxy on InSb (001) substrates at temperatures in the range of 235–295 °C have been studied using conventional and advanced electron microscopy techniques. Defect analysis based on bright-field electron micrographs indicates that the structure grown at 265 °C has the best structural quality of the series, while structures grown at 30 °C lower or higher temperature show highly defective morphology. Geometric phase analysis of the CdTe/InSb interface for the sample grown at 265 °C reveals minimal interfacial elastic strain, and there is no visible evidence of interfacial defect formation in aberration-corrected electron micrographs of this particular sample. Such high quality CdTe epitaxial layers should provide the basis for applications such as photo-detectors and multi-junction solar cells.

1. Introduction

The interest in epitaxial thin films of CdTe (bandgap of 1.51 eV at room temperature) grown by molecular beam epitaxy (MBE) began in the early 1980s [1] because of potential applications in optoelectronic devices (e.g. infrared photo-detectors, solar cells) and as intermediary buffers for the growth of HgCdTe alloys on economic substrates [2]. The use of InSb as a candidate substrate for CdTe growth appears ideal because the two materials are nearly lattice-matched ($|\Delta a|/a \le 5\times10^{-4}$ at room temperature), and they have highly similar thermal expansion coefficients. However, even with the application of Cd/Te flux ratios of greater than 1 during growth, defective interfacial III–VI structures still appear to be formed [3]. Interfacial compounds with different lattice parameters are liable to induce strain at the interface and possibly contribute to the formation of extended defects. Through proper handling of MBE growth parameters such as substrate surface preparation, growth temperature [4], and, most importantly, introduction of an intermediate InSb buffer layer in a dual-chamber MBE system [5], epitaxial CdTe films with high structural quality have recently been obtained [6]. One remaining complication for CdTe growth on InSb lies in the fact that CdTe (II–VI compound) and InSb (III–V compound) are heterovalent compound semiconductors. The possible formation of an interfacial III–VI alloy region due to inter-diffusion has been investigated by soft X-ray photoelectron spectroscopy (XPS) [7] and Raman spectroscopy [8]. However, there have so far been no published electron microscopy observations of any such interfacial compounds.

The characterization by X-ray diffraction (XRD) of epitaxial CdTe films grown on InSb substrates at different substrate temperatures has indicated that the full-width at half-maximum value of the CdTe XRD peak may not be a strong indication of the structural quality [9]. Thus, alternative techniques such as photoluminescence and cross-sectional transmission electron microscopy (XTEM) need to be combined to provide a more comprehensive characterization of the CdTe epilayer. In this study, conventional and aberration-corrected TEM imaging have been used to characterize the structural quality of epitaxial CdTe/$Mg_xCd_{1-x}Te$ ($x\sim0.24$) double heterostructures grown on (001) InSb substrates with intermediate InSb and CdTe buffer layers. The strain distribution across the CdTe/InSb interface has also been investigated using the technique of geometric phase analysis [10].

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2. Experimental details

The specimens under investigation were grown in a dual-chamber VG V80H MBE system with separate III–V and II–VI chambers connected by an ultrahigh-vacuum (UHV) transfer chamber. A schematic of the as-grown structures is shown in Fig. 1. First, InSb buffer layers of 500-nm thickness were grown on InSb (001) substrates in the III–V chamber. Monitoring *in situ* using reflection high-energy electron diffraction (RHEED) confirmed that the InSb surface oxide had been completely removed and that the InSb buffer layers had excellent crystallinity. The quality of the InSb buffer layers in all cases was later confirmed in the XTEM images. The wafers were then transferred to the II–VI chamber under UHV to receive Cd flux treatment prior to CdTe growth to suppress the possible extensive formation of interfacial III–VI compound. The Cd/Te flux ratio during growth was kept fixed at 1.5:1 after an initial two-minute period with a Cd/Te ratio of 3.5:1. RHEED was used throughout to monitor the II–VI growth [6]. As the CdTe growth was initiated, the RHEED pattern invariably turned hazy during a transition from the InSb to the CdTe pattern. At low substrate temperature (235 °C), the transition to clear 2×1 and $c(2\times2)$ patterns, which were used to confirm the Cd-rich condition, occurred quite rapidly compared with the growths done at higher temperature. After growth of the 500-nm-thick CdTe buffer layer, the CdTe/$Mg_xCd_{1-x}Te$ double heterostructure was grown, with the 1-μm-thick CdTe film sandwiched between two 30-nm-thick $Mg_xCd_{1-x}Te$ barrier layers with nominal Mg composition of 24%. The growth temperature was systematically varied (235 °C, 265 °C and 295 °C) while all other growth conditions were kept fixed.

Because of the known sensitivity of CdTe to argon-ion-milling [11,12], precautions need to be taken to ensure that the microstructure of CdTe epilayers observed via TEM is representative of the as-grown structure. Hence, argon-ion-milling should be performed using a liquid-nitrogen-cooled specimen holder [11,13]. Moreover, adequate thickness of the thinned film should be maintained prior to final milling to eliminate plastic deformation induced during post-growth mechanical polishing [14]. Most samples observed here were prepared for TEM observation along ⟨110⟩-type projections using traditional mechanical polishing and dimple grinding, followed by argon-ion-milling (maximum beam energy 2.2 keV) under liquid-nitrogen cooling in an effort to reduce ion-beam damage. One sample was prepared using low-voltage focused-ion-beam milling followed by ion-beam cleaning at 500 eV using a Fischione NanoMill. Electron microscopy was performed using a JEOL JEM-4000EX high resolution electron microscope with an accelerating voltage of 400 kV and structural resolution of 1.7 Å, and an aberration-corrected FEI-Titan 80–200 (scanning) transmission electron microscope (STEM) with sub-Å resolution remotely operated at 200 keV. Geometric phase analysis (GPA) was applied to the as-recorded aberration-corrected high-angle annular dark-field (HAADF) STEM images using a dedicated script in order to extract information about the strain distribution across the CdTe/InSb interfaces [15].

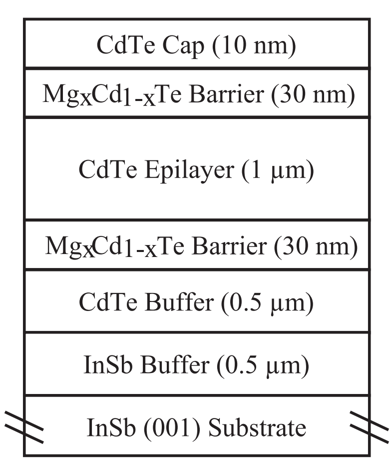

Fig. 1. Schematic (not to scale) showing the CdTe/$Mg_xCd_{1-x}Te$ double heterostructure, as grown on (001) InSb substrate, with intermediate InSb buffer, CdTe buffer and capping layers.

3. Results and discussion

Growth temperature had a major impact on the film morphology. As shown in the bright-field (BF) XTEM image in Fig. 2(a), many dislocations and threading defects were present in the lower part of the film grown at 235 °C, both in the CdTe buffer and also in the CdTe/$Mg_xCd_{1-x}Te$ double heterostructure regions. Most defects seemed to originate at or near the CdTe/InSb buffer interface, although there was no evidence for any Te precipitates, and the defect density dropped off considerably as the growth continued. Fig. 2(b) is a representative image showing the upper part of the heterostructure, and much less defects are visible in this region. Defect densities were estimated from the cross-sectional electron micrographs to range from $>10^9\ cm^{-2}$ near the CdTe/InSb interface to ~mid-$10^7\ cm^{-2}$ near the top surface. Ion-milling damage in CdTe has been identified previously as consisting primarily of planar-faulted dislocation loops with a density that is independent of sample thickness along the electron beam direction [11,16]. This is clearly not the situation here since the defect density steadily decreases moving away from the substrate.

Similar highly-defective film morphology was also observed for the structure grown at 295 °C as shown in Fig. 3. The bottom part of

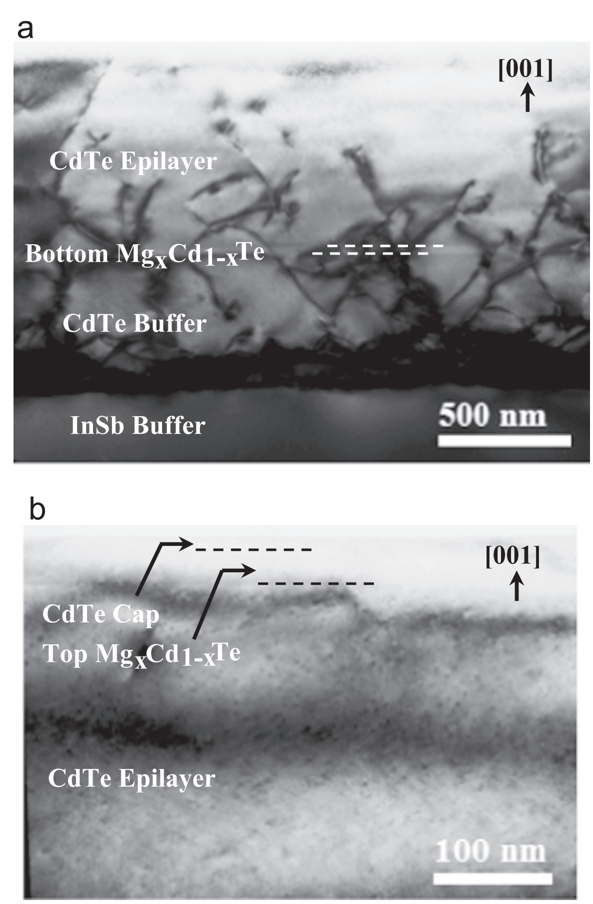

Fig. 2. BF XTEM images of the CdTe/$Mg_xCd_{1-x}Te$ double heterostructure grown at 235 °C: (a) lower region (close to the substrate); (b) upper region.