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Molecular beam epitaxial re-growth of CdTe, CdTe/CdMgTe and CdTe/CdZnTe double heterostructures on CdTe/InSb(1 0 0) substrates with As cap

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ABSTRACT

Molecular beam epitaxial growth on CdTe substrates is challenging since the CdTe film crystalline and optical quality is limited by residual defects including threading dislocations and stacking faults. This remains an obstacle in spite of exhausting variables including pre-growth substrate preparation as well as epitaxial growth conditions including thermal oxide desorption, growth temperature, and II/VI flux ratios. We propose a new technique to re-grow structures with low defect densities and high optical and structural quality on InSb substrates. The “CdTe virtual wafer” is made by growing a thin CdTe film on an InSb(1 0 0) substrate which is then covered with a thin As cap layer to prevent oxidation of the CdTe surface. The As cap can be removed by thermal desorption at about 300 C leaving a clean CdTe surface for subsequent epitaxial growth. This method eliminates the need for chemical etching of CdTe substrates which has been found to lead to an atomically rough surface with residual Carbon and Oxygen contamination. XRD and SEM characterization show a smooth transition from the buffer CdTe to re-grown CdTe layer with identical crystalline quality as for virtual wafer. Steady-state PL and time-resolved PL from CdTe/CdMgTe double heterostructures show substantial improvement in luminescence intensity and carrier lifetime comparable to values for identical samples grown without exposure to atmosphere. We will also report on CdTe/CdZnTe double heterostructures grown on virtual wafers compared to identical structures on conventional CdTe(2 1 1)B substrates.

1. Introduction

In CdTe-based solar cells, it is critical to have a low defect density absorber material to enhance minority carrier lifetime. Modeling studies have shown that single crystal CdTe solar cells have a potential to achieve efficiencies over 25% [1]. In order to enhance CdTe solar cell efficiency, it is necessary to increase the minority carrier lifetime as well as absorber carrier density [2]. The electrically-active absorber carrier density is directly correlated to material defect density [3,4]. These defects are as form of dislocations, twins, and anything else non-radiative, but they predominantly appear to be dislocations. In this work, we show how to significantly reduce defect densities and demonstrate the growth of test structures with high minority carrier lifetime in CdTe epitaxial films.

There have been extensive attempts to grow molecular beam epitaxial (MBE) CdTe films on CdTe substrates using different crystal orientations over a range of substrate temperature and Cd/Te flux ratio to improve the crystalline quality and reduce defect density. However these efforts have resulted in limited success and cannot reduce defect density below approximately $1 \times 10^6\,cm^{-2}$ using currently available commercial CdTe substrates. Fig. 1 shows confocal photoluminescence (c-PL) images for a series of samples including a 1 μm thick CdTe grown on single crystal CdTe(2 1 1)B substrate. The Cd/Te flux ratio is one and is derived from direct thermal decomposition of CdTe using a single effusion cell. The substrate temperature was varied from 250 C to 300 C. Identical samples with different Cd/Te flux ratio in a range of 1.0 to 1.4 using an additional Cd effusion cell have also shown a similar trend with defect density values not less than $1 \times 10^6\,cm^{-2}$. Table 1 shows a

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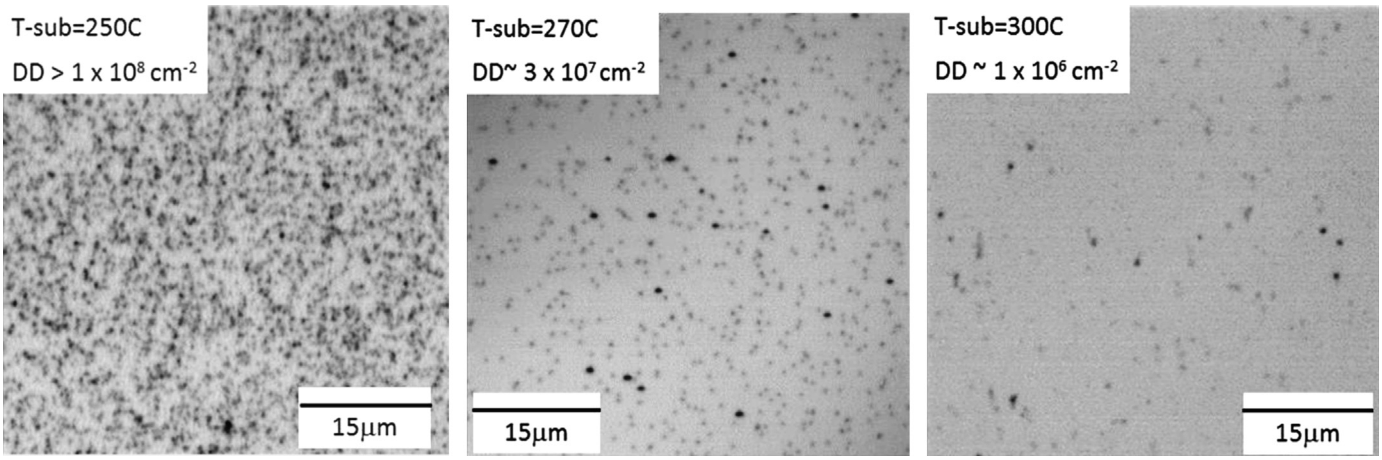

Fig. 1. Confocal PL images from buffer CdTe layer grown on CdTe(2 1 1)B substrates, showing correlation between defect density and substrate temperature at constant Cd/Te ratio of one.

Table 1
Defect density as a function of optimized CdTe growth condition on CdTe(2 1 1)B substrate. In best growth condition, defect density does not decrease below 10^6 cm^{-2}.

		Substrate temperature (C)		
		250	270	300
Cd/Te ratio	1.0	1×10^8	3×10^7	1×10^6
	1.2	2×10^7	3×10^7	5×10^6
	1.4	1×10^8	1×10^8	3×10^7

summary of defect density values for the whole matrix. These residual defect densities limit the minority carrier lifetime and optical characteristics of any structures grown on these CdTe wafers.

2. Experimental procedure

The growth of CdTe-on-InSb is carried out in two separate III–V and II–VI MBE chambers which are connected by a UHV transfer chamber. In the first step, an InSb buffer layer of about 600 nm is grown in the III–V chamber which is then transferred in-vacuo to the II–VI chamber to grow an epitaxial CdTe buffer layer. In the second step, the wafer is transferred back to the III–V chamber to deposit a thin As cap layer to protect the CdTe surface from oxidation. The next step of epitaxial growth can be performed either in this chamber or in an ex-vacuo II–VI MBE chamber. Crystalline and expitaxial quality were examined by rocking curve XRD and plan-view and cross-section SEM. Optical quality of the samples was measured by room temperature photoluminescence (PL) with a 660 nm excitation laser. Defect densities were measured using a laser scanning confocal photoluminescence (c-PL) system with a 0.25 μm resolution. Time-resolved photoluminescence (TRPL) was used to determine carrier lifetime.

2.1. Epitaxial re-growth of CdTe on CdTe/InSb(1 0 0) virtual wafers

MBE growth of CdTe on InSb(1 0 0) has been shown to be promising due to very small lattice mismatch between these two binary semiconductors [5] and easier surface preparation of InSb substrates. c-PL and XRD measurements show a high crystalline quality with low defect density in the re-grown CdTe layers on these substrates.

We consider two different methods to prepare the CdTe/InSb substrates before re-growth of the next CdTe layer. In the first approach, the sample is dipped in a diluted HCl mix with DI water, followed by a sequence of DI water and Methanol rinse. The sample was then transferred into the MBE chamber where CdTe growth was performed after thermal desorption of the native oxide. This growth is determined to be epitaxial as the XRD from the CdTe layer lies over the CdTe peak from the starting CdTe/InSb(1 0 0) substrate, as indicted in Fig. 2(b). The peak broadening however indicates a degraded crystalline quality for the top CdTe layer. In fact, the interface between two CdTe layers is readily observable by cross-section SEM image shown in Fig. 2(a). We could improve the second CdTe epitaxial layer growth to obtain comparable crystalline quality to the starting CdTe/InSb wafer by optimizing chemical etch step and in-situ heat treatment for oxide desorption. However this process was not well repeatable in a series of identical growth runs.

In the second approach, we utilized the CdTe/InSb which included a 10 nm As cap layer to protect the CdTe surface from oxidation in atmosphere. The "CdTe virtual wafers" are prepared by growth of an InSb buffer layer on InSb(1 0 0) substrate in a III–V MBE chamber. The wafer is then transferred in-vacuo to the second II–VI MBE chamber for growth of CdTe buffer layer. The wafer is finally transferred back to the III–V MBE chamber for deposition of the As cap layer. This virtual wafer can be exposed to atmosphere at this point and stored in a N2 purged desiccator for subsequent epitaxial growths. A virtual wafer is then loaded into another MBE chamber for re-growth of a II–VI structure. Before MBE growth, the substrate is annealed at 300 C for 15 min to thermally desorb the oxidized As cap layer. No wet chemical treatment step is applied in this process.

Fig. 3(a and b) shows top view as well as cross-section image of the CdTe layer grown on a virtual wafer, after As desorption. No interface is observed between CdTe layer from the virtual wafer and the second epitaxial layer of CdTe indicating a clean transition between the two separately grown CdTe layers. The smooth top surface is comparable with the surface quality of the CdTe virtual wafer with no As cap layer. Fig. 3(c) shows the XRD from this sample. The peak from CdTe lays directly over the one from the virtual wafer with comparable FWHM indicating high crystalline quality of the second epitaxial CdTe layer. The average defect density measured by c-PL of the CdTe epitaxial layer grown on such a virtual substrate is in the low 2×10^5 cm^{-2}. One of the c-PL images is shown in Fig. 4 indicating a local defect density of less than 4×10^4 cm^{-2} as no defect was observed in this region of sample.

2.2. Epitaxial re-growth of CdTe/CdMgTe and CdTe/CdZnTe double heterostructures on CdTe/InSb(1 0 0) virtual wafers

Ternary II–VI group semiconductors have been studied in the past as electronic barrier material to confine carriers in CdTe due

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