Effect of target–substrate separation on HgCdTe films formed by pulsed laser deposition

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ABSTRACT

HgCdTe thin films were deposited on Si (1 1 1) substrates at different target–substrate separations by pulsed laser deposition (PLD). The results show that the kinetic energy of the incident particles, and the thickness, crystallinity, elemental composition and surface morphology of the HgCdTe thin films are affected by the change of the target–substrate separation. The HgCdTe films prepared using Nd:YAG laser show cubic phase. The films prepared by PLD on the undoped Si substrates can form $SiTe_4$ between the HgCdTe film and the Si substrate at small target–substrate separation distance. The formation of interfacial Si–Te may affect the quality of PLD HgCdTe thin films on Si substrates.

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1. Introduction

Mercury cadmium telluride (MCT, $Hg_{1-x}Cd_xTe$) thin films are important materials for many infrared focal plane array (FPA) applications because of the variable band gap, depending on Hg composition, which provides unprecedented freedom in infrared (IR) detector design [1]. Several candidates such as Si, GaAs, sapphire and InSb have been studied as alternative substrates in the HgCdTe field. Among these candidates, the best one is silicon, because it is the best window material in both mid- and long-wave IR range, and it is the best material for larger area substrates [2]. If HgCdTe could be directly grown on Si substrates, it would be advantageous for the fabrication of large FPAs [3].

At present, many methods have been used to produce the HgCdTe thin films, such as molecular beam epitaxy (MBE) [4], metal-organic chemical vapor deposition (MOCVD) [5], etc. Compared to these epitaxial methods, pulsed laser deposition (PLD) is a very promising technique [6]. Many research groups have obtained HgCdTe thin films by this method [7–9], and have investigated the effects on the different technological aspects and properties of PLD HgCdTe thin films, such as different Si substrates [10], substrate temperature [11], electrical properties [10], crystalline properties [11,12], etc. The quality, compositions and crystallographic orientations of HgCdTe thin films obtained by PLD depend strongly on the parameters during deposition.

However, the influences of the target–substrate separation distance on the properties of HgCdTe thin films have not been complete. It is an important aspect which influences the properties of HgCdTe thin films, and very important for growing high quality alloy thin films using PLD. In the present paper, the HgCdTe thin films were grown by PLD on undoped Si at different target–substrate separation distance (35–55 mm). The properties of HgCdTe thin films were investigated by scanning electron microscope (SEM), atomic force microscope (AFM), energy dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD) and selected area electron diffraction (SAED).

2. Experiment

The HgCdTe thin films were deposited on undoped Si (1 1 1) substrates using a Nd:YAG laser with a wavelength of 1064 nm, a pulse duration of 10 ns and a repetition rate of 10 Hz. The schematic representation of the experiment has been shown in our previous work [13]. Crystalline $Hg_{1-x}Cd_xTe$ ($x=0.2$) was used as a target. The deposition time was 10 min. The Ar partial pressure was kept at 5×10^{-3} Pa by adjusting the flow rate of the Ar gas. The substrate temperature was 200 °C. During the deposition, the laser incident energy was kept at 200 mJ. The target–substrate separation distance (D_{t-s}) was varied from 55 to 35 mm.

The film thickness was measured from a cross-sectional image obtained by SEM using a Hitachi S-570 microscope. The surface

morphologies were obtained by a PARK Autoprobecp AFM measurement. The composition of the HgCdTe thin films was analyzed by EDS using a JXA-8800R electron probe micro-analyzer (EPMA). Rigaku D/max-rB XRD spectroscopy with a Cu Kα line radiation source was used to characterize the structure of the HgCdTe thin film. A standard θ–2θ scanning method was employed in the XRD for the crystallographic phase analysis and determination of the preferential orientation of the deposited films. Plan-view SAED patterns were carried out by a Hitachi H-800 transmission electron microscope (TEM) system.

3. Results and discussion

3.1. Thickness and AFM results

Fig. 1(a)–(e) presents the SEM cross-sectional images of the HgCdTe thin films deposited at different D_{t-s}. The film thickness increases with the decrease of D_{t-s}. The surface morphologies of HgCdTe films on Si (1 1 1) substrates at different conditions are shown in Fig. 2. The images are measured over 15 μm × 15 μm scanning ranges. The surface root-mean square (RMS) roughness values of the films deposited at different D_{t-s} are 8.29 (55 mm), 8.16 (50 mm), 6.99 (45 mm), 5.50 (40 mm) and 12.20 (35 mm) nm, respectively. The film surface image shown in Fig. 2(a) is very rough and the grain boundary is indistinct. With decreasing D_{t-s}, some crystalline grains with distinct boundaries appear, and the surface of the film becomes smooth. At D_{t-s}=35 mm, some large grains appear and the film surface becomes rough again.

In inert gas ambient, the particles in the plasma collide and exchange energy with gas molecules. The kinetic energy of the particles in the plasma decrease with the increase of the plasma expansion scale. At the largest separation distance (D=55 mm), the fewest particles reach the substrate due to a lower flux density. Some small grains may form before arriving at the substrate surface. A few atoms arriving at the substrate have low kinetic energy. The probability of incident atoms moving on the surface of the substrate is very small. Therefore, the growth orientation and shape of the crystallites are random, and the

surface is very rough. With the decrease of D_{t-s}, the number and kinetic energy of the incident atoms arriving at the substrate increase. The proportion of the atoms combining with each other before reaching the substrate surface will decrease. A large population of small crystalline grains and only a few large grains are present on the film surface. The surface becomes smooth, and the thickness of the films becomes large. But when D_{t-s} is less than 40 mm, many large particles, drops and clusters have no time to be decomposed completely and arrive at the substrate surface indirectly, which causes the shadow effect in the films. Meanwhile, a lot of incident atoms are re-sputtered because of their higher kinetic energy. Some holes left in the film cause the film thickness to increase and affect the surface quality of the films.

4. Composition and XRD results

Fig. 3 shows the EDS results of HgCdTe film stoichiometry obtained at different target–substrate separation distances. EDS is an important method that provides the information about the chemistry of the thin film. The results show that the samples only include Hg, Cd and Te in the films. At D_{t-s}=50 mm, the composition of the film is close to that of the target (x=0.2), while the films deposited at other D_{t-s} are Cd-rich. In reducing D_{t-s} from 50 to 35 mm, both the Hg and Cd content of the film decrease, while the Te content increases. At D_{t-s}=35 mm, the Hg content is very low, even lower than that of the Cd content.

Fig. 4 shows the XRD patterns of HgCdTe thin films deposited at different conditions. The XRD peaks at around 2θ=28.4° and 2θ=58.9° are attributed to Si substrate, and other main peaks denoted with a "○" in Fig. 4 are corresponding to HgCdTe planes. Two strong peaks appearing at 2θ=23.8° and 2θ=39.4° correspond to the (1 1 1) plane and (2 0 0) plane of HgCdTe thin films, respectively. At D_{t-s}=55 mm, the crystalline quality of the HgCdTe thin films is poor. With decreasing D_{t-s} from 50 to 35 mm, the intensity of the HgCdTe diffraction peaks becomes strong with the decrease of D_{t-s}. This is related to the thickness of the film. The lattice constant of HgTe is very similar to that of CdTe ($\Delta a/a$=0.3%). HgCdTe is a pseudo binary compound, $(HgTe)_{1-x}$
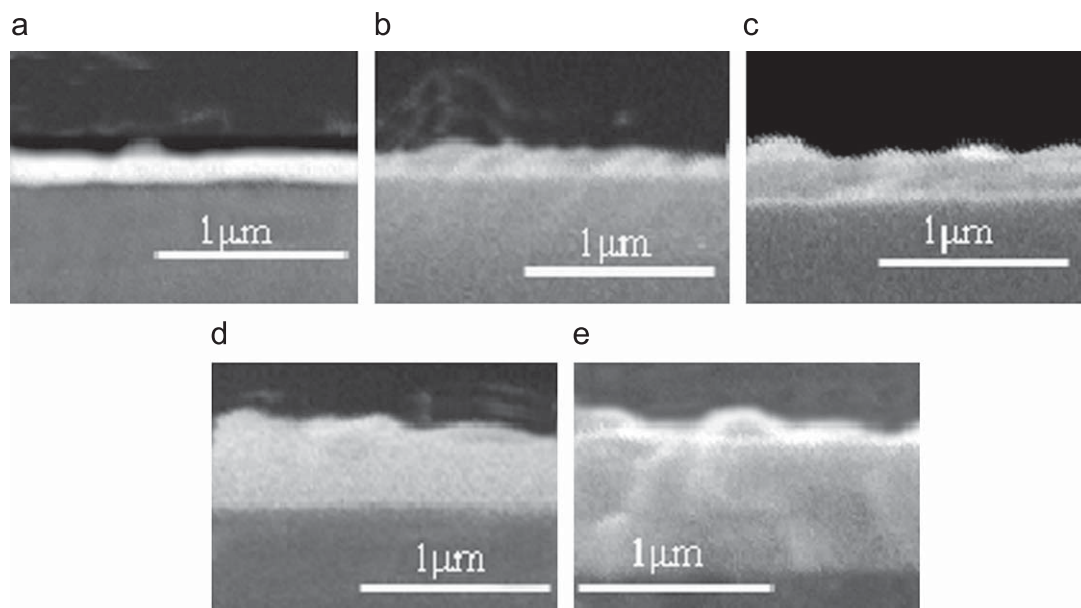

Fig. 1. The thickness of HgCdTe thin films deposited at D_{t-s}=(a) 55 mm, (b) 50 mm, (c) 45 mm, (d) 40 mm, (e) 35 mm.
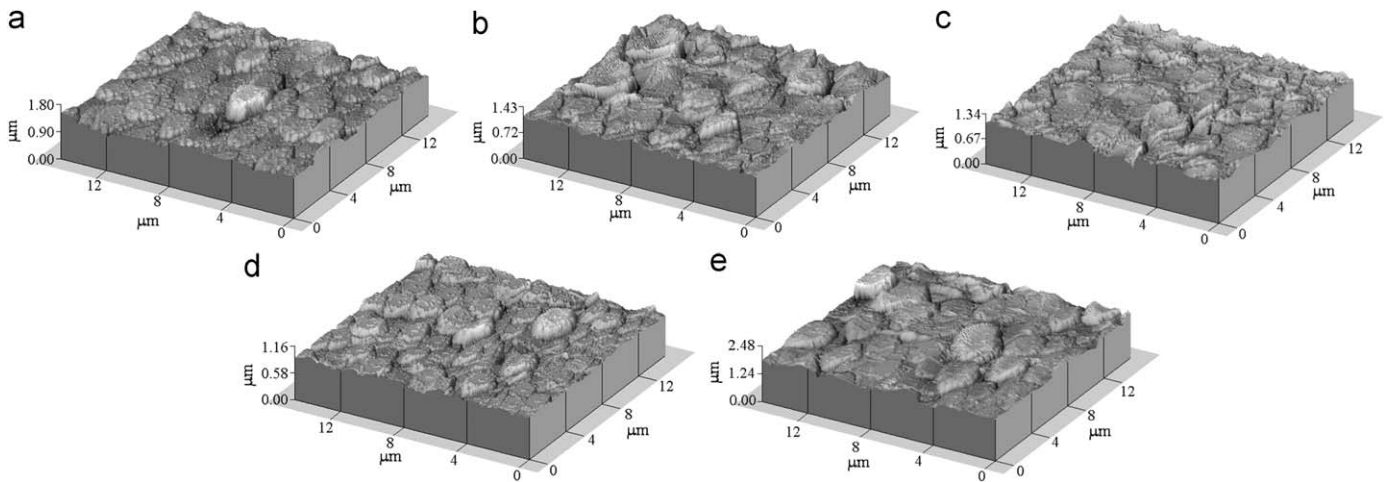
Fig. 2. AFM images of the HgCdTe thin films deposited at s D_{t-s}=(a) 55 mm, (b) 50 mm, (c) 45 mm, (d) 40 mm and (e) 35 mm, respectively.
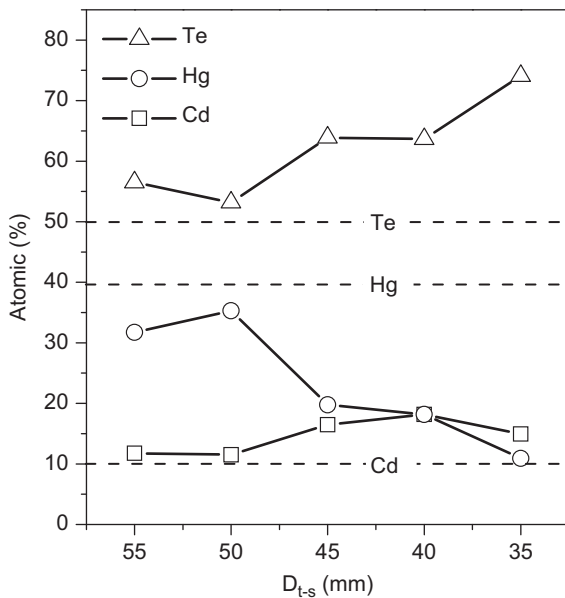

Fig. 3. Concentration variation of Hg, Cd and Te for the HgCdTe films deposited at different D_{t-s}. Dashed line shows the elemental composition of the target.
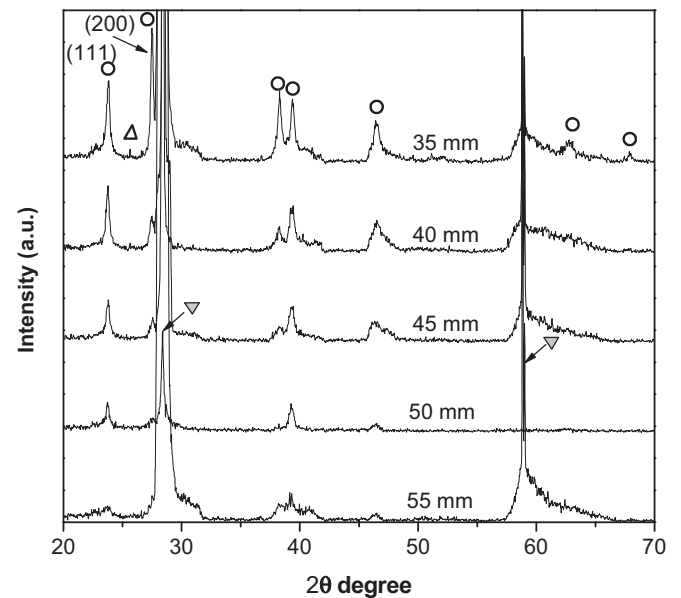

Fig. 4. Comparison of XRD patterns of HgCdTe thin films deposited at different D_{t-s}. The "○" denotes the main peaks corresponding to HgCdTe planes, the "△" denotes the SiTe$_4$ (1 0 0) peak and the "▽"denotes the Si substrate.

$(CdTe)_x$, with arbitrary proportion. But compared powder diffraction file (PDF, 150770, CdTe) with PDF (320665, HgTe) carefully, HgTe contains (2 0 0) peak, but CdTe does not. The (2 0 0) peak is an evidence that there are HgTe crystallites in the film. The existence of HgCdTe film obtained at these conditions can be confirmed by the presence of CdTe crystallites and HgTe crystallites. The (1 1 1) plane is the lowest energy plane of the face-centered cubic (fcc) structure. Thus the HgCdTe films prepared using Nd:YAG laser with these conditions show cubic phase. When D_{t-s} was decreased to 35 mm, the intensity of (2 0 0) peak is stronger than that of (1 1 1) peak. This means that the thin film contains more and more HgTe crystallites with decreasing D_{t-s}. Furthermore, there is one weak peak at 2θ=25.64° appearing at D_{t-s}=40 mm and D_{t-s}=35 mm. It is corresponding to the (1 0 0) plane of SiTe$_4$. Combined with the result of the EDS, the Te atoms may react with the Si atoms on the substrate and form an interlayer between the substrate and the HgCdTe epitaxial layer.

The structure of HgCdTe films is further evidenced by the plan-view SAED patterns shown in Fig. 5. The patterns of the film
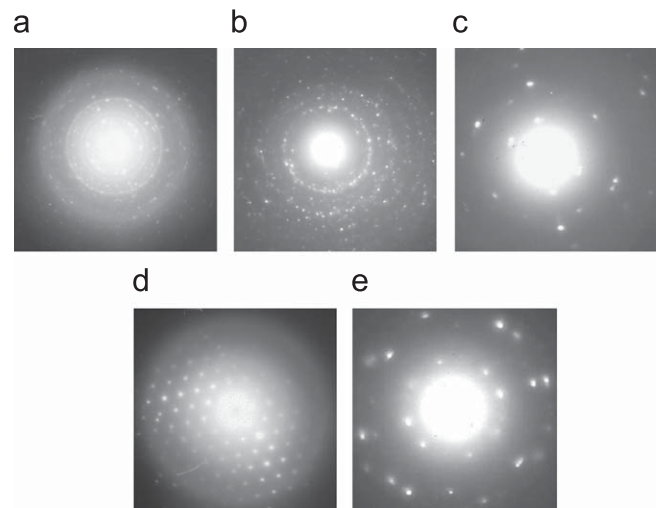

Fig. 5. Plan-view SAED patterns of the HgCdTe thin films deposited on Si(1 1 1) at (a) 55 mm, (b) 50 mm, (c) 45 mm, (d) 40 mm and (e) 35 mm.

deposited at D_{t-s}=55 mm shows the halo rings, suggesting an amorphous structure. Weak diffraction spots (Fig. 5(b)) point out minor orientation of crystallites. In reducing D_{t-s} from 45 to 35 mm, the films have a more crystalline structure.

The crystalline quality and the composition of the film have a relation to the kinetic energy of the incident atoms. As is known, the velocity of different kinds of atoms is different when they leave the target surface ($V_{cd} > V_{Te} > V_{Hg}$) [14]. In gas ambient, the ablated atoms will collide with the gas molecules. The atoms with a large velocity will encounter a large resistance. As a result, the kinetic energy of Hg atoms is more than that of Cd atoms when they arrive at the substrate surface at the same time, especially in a large D_{t-s}. When D_{t-s} is large (55 mm), all kinds of atoms arriving at the substrate have a low kinetic energy. The atoms are absorbed on the substrate surface only by physical adsorption and do not move randomly. The probability of different atoms combining with each other is very small. Thus the growth orientation of the atoms is random and crystalline quality is poor. At this condition, the number of chemical bonds is small. The atoms adhere to the surface only through the van der Waals force. While the van der Waals force of the Hg atoms is smaller than that of Cd atoms. A few Hg atoms may be desorbed from the film. At D_{t-s}=50 mm, the kinetic energy of the incident atoms increases. The combination probability of Hg, Cd and Te atoms increases. The increase of the chemical adsorption in the film prevents the Hg atoms evaporating from the film. The composition is close to that of the target. But the atoms have not enough kinetic energy to form the crystallites growing with definite crystal orientations. The crystalline quality is not obviously improved. With reducing D_{t-s} from 45 to 35 mm, the atoms have enough energy to move quickly to look for the appropriate sites, combine with each other and form the crystalline HgCdTe film. CdTe is ionic compound, while HgTe is semimetal. The bond energy of Cd–Te is stronger than that of Hg–Te. Thus, the large incident kinetic energy will cause the Hg atoms to be sputtered from the film surface more easily than the Cd atoms. The Hg vacancy defects present in the film. The Hg composition of the thin films descends quickly with the decrease of D_{t-s}. Some Te atoms approaching the substrate may combine with the Si atoms of the substrate and form SiTe$_4$. The radii of the two ions Te^{1+} and Si^{4-} are 0.82 and 2.71 Å, respectively, and the radius ratio $r_{Te^{1+}}/r_{Si^{4-}} = 0.302$, the value is in the range 0.225–0.414. It can be deduced that the Si and Te ions in the interlayer exhibit tetrahedral bonding, similar to that observed in HgCdTe and Si. The formation of SiTe$_4$ is the first reported on HgCdTe thin film on Si substrate prepared by PLD. Moreover, the interlayer only forms when the incident atoms have a large kinetic energy. The stable chemical bond formed between Si and Te may affect the quality of the HgCdTe thin films, and this conclusion needs to be further confirmed later. At D_{t-s}=35 mm, the incident atoms have a very high kinetic energy. The incident atoms can move on the substrate quickly and randomly, and form the crystallites growing with different crystal orientations. The relative intensity of the HgTe (2 0 0) and other peaks becomes strong.

5. Conclusion

The effect of the D_{t-s} on the properties of HgCdTe thin films on Si substrates deposited by PLD were investigated in this paper. It was found that the HgCdTe film properties such as crystalline quality, elemental composition and surface morphology properties have a strong relation to the change of D_{t-s}, and the HgCdTe films prepared using Nd:YAG laser show cubic phase. It may be possible to obtain PLD HgCdTe thin films adapted for IR sensing of various wavelengths. An analysis of the experiment results indicates that the SiTe$_4$ can present between the HgCdTe film and the Si substrate at the small D_{t-s}, which may affect the quality of the HgCdTe thin films grown on Si substrates.

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