



Proceedings Diffusion of Dopants and Components in Arsenic-Implanted CdTe/HgCdTe Structures under Different High-Temperature Annealing Conditions *

Changzhi Shi *, Chun Lin and Yanfeng Wei

Research Center for Advanced Materials and Devices, Shanghai Institute of Technical Physics, Chinese Academy of Sciences, Shanghai 100049, China; chun_lin@mail.sitp.ac.cn (C.L.); yfwei@mail.sitp.ac.cn (Y.W.)

- * Correspondence: shichangzhi@mail.sitp.ac.cn
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Abstract: The CdTe cap layers were grown on CdZnTe-substrated HgCdTe (MCT) LPE epilayers by magnetron sputtering and thermal evaporation. The diffusion behaviors of Cd & Hg components and impurities (As or In) in these CdTe/MCT structures subjected to As ion implantation and various Hg overpressure annealing processes were investigated. The conclusions indicate that the defects at the CdTe/MCT interface could produce the accumulations of impurities and the distributions of induced damages (related to the cap layer structure) have a significant influence on the diffusion of components and impurities. By adjusting annealing procedures, the diffusions of components and impurities can be controlled.

Keywords: HgCdTe; CdTe; arsenic-implanted; diffusion; annealing; component; impurity

1. Introduction

So far, HgCdTe (MCT) remains to be an irreplaceable infrared (IR) sensing material with a tunable energy gap by varying Cd component, covering the entire IR spectra (from NIR to VLWIR), despite the challenges from type-II superlattice, quantum well (QW) and even two-dimensional materials. It has been extensively applied in the IR detectors and systems with the advantages of high detectivity, rapid spectral response and high quantum efficiency. A critical path to improve the device performance of MCT-based photodiodes is to suppress dark current. Therefore, on one hand, the p-on-n photodiode structure is adopted to reduce bulk dark current [1,2]; on the other hand, the high-quality passivation of MCT surface is required to reduce the surface leakage and recombination current.

The arsenic ion implantation and the post-annealing have been demonstrated to be a feasible roadmap to achieve the p-on-n structure [2]. Accordingly, the dislocations and defects at the interface between the passivation layer and the MCT epilayer originating from lattice mismatch have to be healed or reduced to acquire a good surface passivation. In order to suppress the effect of interface dislocations, the graded-gap layer is grown on the MCT epilayer. The studies on the structure changes of the graded-gap MCT epilayers after ion implantation and annealing were reported [3,4]. Furthermore, the influence of post-annealing on the re-structuring of arsenic-implanted (at a low implant energy of <200 keV) MCT epilayer coated with in-situ graded-gap layer by molecular beam epitaxy (MBE) was investigated [5]. With the development of passivation technique, the film deposition method, such as atomic layer deposition (ALD), was utilized to prepare passivation layer (Al₂O₃) on uneven MCT device surface. Nevertheless, the research result indicates that a graded-gap CdTe intermediate layer is needed to be grown between the mismatched upper passivation layer and the MCT bulk epilayer to reduce slow and fast surface

states [6]. Thus, the formation of graded-gap CdTe layer on MCT epilayer is significant for the acquisition of high-quality surface passivation. In our previous work [7,8], the influences of CdTe and ZnS cap layer microstructures on the implanted ion distributions and diffusions in MCT epilayers were studied. Here, the research work is focused on the CdTe/MCT structures, which is prepared by depositing CdTe cap layers onto MCT substrates by magnetron sputtering and thermal evaporation. Then, the graded-gap CdTe layers were achieved by the component interdiffusion between CdTe and MCT under Hg overpressure annealing, and the diffusion behaviors of Cd & Hg components and As & In impurities in these structures through As ion implantation and different Hg overpressure annealing conditions were characterized by SIMS and TEM. Finally, the roles of

2. Materials and Methods

2.1. Epilayer and Cap Layer Growth

The MCT epilayers were grown on CdZnTe (111) substrates by LPE. Then, the CdTe cap layers were prepared on the MCT samples through magnetron sputtering (MS) and thermal evaporation (TE) as illustrated in Table 1.

the cap layer structures and induced damages on these behaviors are discussed.

Table 1. Parameters of cap layer growth, arsenic ion implantation, Hg overpressure annealing (pre-annealing, activation annealing and post-annealing) for CdTe/MCT structure samples.

Sample	Cap Layer	Pre-Anneal	As Ion Implant	Cap Layer Preservation	Activation Annealing	Post-Anneal Cap Layer	Post-Annealing
A1	MS	240 °C	No	Yes	No	No	No
A2	TE	240 °C	No	Yes	No	No	No
B1	TE	No	Yes	Yes	420 °C 1.5 h + 24 0°C	No	No
B2	TE	No	Yes	No	420 °C 1.5 h + 240° C	No	No
C1	TE	240 °C	Yes	Yes	420 °C 1.5 h + 240 °C	No	No
C2	MS	240 °C	Yes	Yes	420 °C 2 h + 240 °C	No	No
C3	TE	240 °C	Yes	Yes	420 °C 2 h + 240 °C	No	No
D1	TE	240 °C	Yes	No	420 °C 1 h + 240 °C	TE	420 °C 0.5 h + 240 °C

2.2. Ion Implantation and Annealing

The technological processes of pre-annealing, ion implantation, activation annealing, post-annealing cap layer deposition and post-annealing for CdTe/MCT samples are provided in Table 1. All the annealing processes were performed under Hg vapor overpressure. Group A samples without ion implantation are pre-annealed at 240 °C to demonstrate the diffusion of components and indium dopants in MCT covered by different cap layers under Hg overpressure pre-annealing. The implant conditions for all ion implanted samples (Group B, C and D) are implant energy = 350 keV and implant dose = 1×10^{14} cm⁻², and the activation annealing was carried out in two temperature steps of 420 °C (for p-type activation of As ions) and 240 °C (for elimination of residual Hg vacancies). In order to investigate the diffusion of components and its influence on the diffusion of implanted As ions during activation annealing, the cap layer in Sample B1 was preserved, while the cap layer in Sample B2 was removed before activation annealing. The CdTe/MCT structures in Group C and Sample D1 were pre-annealed at 240 °C to obtain interdiffusion of Cd component between cap layer and MCT. The difference between Group C and Sample D1 is that the pre-annealed cap layer was removed before activation annealing and the post-annealing cap layer was grown and post-annealed to acquire component interdiffusion heterostructure for Sample D1.

2.3. Measurement and Characterization

The secondary ion mass spectroscopy (SIMS) is used to acquire the distribution profiles of components (Cd, Hg) and impurities (As, In) in the CdTe/MCT samples. The cross-section

micro-structure images of the above samples were characterized by transmission electron microscopy (TEM) in bright-field mode. In order to obtain the TEM samples, the original samples were cut into thin sheets, and then these sheets were polished chemically and thinned by ion milling to less than 100 nm. In the Hall effect measurement, the samples were thinned from the back by the chemical etching of bromine etchant and then measured using Hall effect tester at 77 K layer by layer. Finally, the activation rates of As ions in the annealed samples can be calculated with the As concentrations from SIMS profiles and the differential carrier concentrations from Hall effect test.

3. Results and Discussion

3.1. Interdiffusion without Ion Implantation

The diffusion profiles of Cd & Hg components and indium dopants in MS-CdTe/MCT and TE-CdTe/MCT structures after pre-annealing at 240 °C are illustrated in Figure 1. The thicknesses of Cd diffusion layers in A1 and A2 are both ~160 nm. Moreover, the outdiffusion of indium dopants occurs to these two samples. However, it is noteworthy that the outdiffused indium dopants are accumulated at the interface of CdTe/MCT in A2, which is likely due to the higher defect density at the TE-CdTe/MCT interface than the MS-CdTe/MCT interface. The high density of defects at the TE-CdTe/MCT interface hinders the successive outdiffusion of indium.



Figure 1. SIMS profiles of Cd & Hg components and indium dopant concentration in CdTe/MCT structures after Hg overpressure annealing at 240 °C for 48hrs: (**a**) The CdTe cap layer was grown by magnetron sputtering; (**b**) The CdTe cap layer was grown by thermal evaporation.

3.2. Interdiffusion with Ion Implantation

Figure 2 provides the diffusions of Cd and Hg components and the distribution profiles of the implanted As ions in Sample B1 and B2. The concentration of 1×10^{15} cm⁻³ is selected as the benchmark lower limit of As ion concentrations. Considering the loss of As ion source by removing the cap layer in B2, the diffusion depths of As ions relative to the CdTe/MCT interface for Group B are 1.2~1.3 µm, which indicates that the diffusions of Cd and Hg components have no significant role on the diffusion of As ions. The activation rate of As ions is estimated to be 30~40% by differential Hall effect measurements.

Compared to Sample B1 without pre-annealing, Sample C1 with pre-annealing possesses a similar diffusion depth of Cd component as shown in Figure 3a. Nevertheless, the diffusion depth of As ions in C1 is ~1 μ m, smaller than that (~1.3 μ m) of B1. From the deeper induced damage distribution in C1 (not provided here), it can be seen that more induced damages near the C1 surface hinder the indiffusion of As ions, and even lead to the accumulation of As ions near the surface. By extending the activation annealing time, the diffusion depth of As ions can stretch to 2 μ m, however, the diffusion of Cd component becomes aggravated as illustrated in Figure 3c. When the MS-CdTe serves as the cap layer, the diffusion depths of Cd component and As ions can be reduced as shown in Figure 3b. Because the MS-CdTe is denser than the TE-CdTe, the pre-annealed cap layer in Sample C2 has better recrystallinity but lower ion blocking ability. It could result in the

deeper distribution of induced damages in C2, thereby reducing the diffusion depths of Cd component and As ions. From the TEM cross-section images of Sample C3 in Figure 3d–g, it can be seen that the amorphized-MCT (a-MCT) and the short defect layer in MCT are eliminated by activation annealing as well as the column structure of the CdTe cap layer. Interestingly, the accumulations of As ions at CdTe/MCT interfaces and in CdTe layer in Figures 2 and 3 could be due to the separation of As precipitates to structural defects, similar to Ref. [9].



Figure 2. SIMS profiles of Cd & Hg components and implanted As ion concentrations in CdTe/MCT structures after Hg overpressure activation annealing at 420 °C and 240 °C: (**a**) The CdTe cap layer was not pre-annealed at 240 °C before activation annealing and preserved during activation annealing; (**b**) The CdTe cap layer was not pre-annealed and removed after ion implantation.



Figure 3. SIMS profiles of Cd & Hg components and implanted As ion concentrations in (**a**) Sample C1, (**b**) Sample C2 and (**c**) Sample C3; (**d**) TEM cross-section image of Sample C3 after activation annealing; (**e**) Column structure of as-grown CdTe cap layer in Sample C3; (**f**) Elimination of column-structured CdTe cap layer after activation annealing; (**g**) Recovery of MCT lattice in Sample C3 by activation annealing.

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In order to avoid the excessive component diffusion, the post-annealing is carried on Sample D1. Figure 4 provides the SIMS profiles of Cd & Hg components and As & In dopants in D1 after post-annealing. The Cd component and As ions have a similar diffusion depth. On the other hand, there is still an accumulation of In dopants at the CdTe/MCT interface. It probably produces the formation of p-layer on the surface. This problem should be resolved in the subsequent work.



Figure 4. SIMS profiles of Cd & Hg components and implanted As ion & indium dopant concentrations in Sample D1.

4. Conclusions

The diffusion behaviors of components and impurities in the CdTe/MCT structures subjected to As ion implantation and Hg overpressure annealing were studied. The diffusion of As ions during annealing is influenced by the distributions of induced damages, which is determined by the structures of the graded-gap CdTe layer on MCT surface. However, the distribution profiles of As ions are not found to be effected by the presence and the removal of CdTe cap layers during Hg overpressure annealing.

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