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***Study of the Diffusion of Te Inclusions in CdZnTe
Nuclear Detectors in Post-Growth Annealing***

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Study of the Diffusion of Te Inclusions in CdZnTe Nuclear Detectors in Post-Growth Annealing

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Abstract—Despite immense endeavor invested in optimizing the crystal growth parameters and the post growth improvement methodologies proposed by numerous studies, there are still unresolved shortcomings of CdZnTe crystals to produce commercial-grade CdZnTe detectors. Post-growth thermal annealing under Zn, Te, or Cd vapor overpressure at various temperature have been the approach attempted to improve the crystallinity of CdZnTe crystals. This paper presents results of post growth annealing of CdZnTe detectors that shows both reduction in the sizes of Te inclusions and the migration of the inclusions towards the high-temperature side of the crystal. Two set of annealing experiments were made. The first is annealing under Cd vapor overpressure in vacuum at 600 °C for 45 minutes at a temperature gradient of 10 °C/cm. The second set of CdZnTe post-growth annealing experiments was carried out at 700 °C CdZnTe annealing temperature with the Cadmium temperature at 650 °C, 30 minutes annealing time, and temperature gradient of 10 °C/cm. The reduction in the sizes of Te inclusions ranges from 8% to 38%.

I. INTRODUCTION

ROOM-TEMPERATURE semiconductor nuclear detector grade materials are desired to have high resistivity (low dark current), high atomic number (good stopping power), good carrier mobility-lifetime product, $\mu\tau$, (for better collection of charge), high band-gap, high crystallinity (uniformity of response), and room temperature performance. Cadmium Zinc Telluride (CdZnTe) is one of the most investigated materials as a wide band-gap semiconductor crystal for nuclear radiation detection [1]–[4], nuclear medicine [5], medical imaging [6], [7], and in the field of astrophysics for measurement of celestial gamma-ray photons [7]. Despite immense endeavor invested in optimizing the crystal growth parameters and the post growth improvement methodologies proposed by numerous studies, there are still

unresolved shortcomings of CdZnTe crystals to produce commercial-grade CdZnTe detectors [8]. Post-growth thermal annealing under Zn, Te, or Cd vapor overpressure at various temperature have been the approach attempted to improve the crystallinity of CdZnTe crystals. One of the widely reported defects is defect associated with Cadmium vacancy created during the crystal growth process. To compensate the Cd vacancy created, eliminate tellurium inclusions and improve the overall performance of the crystal, post-growth thermal annealing of CdZnTe crystals under Cd vapor overpressure has been a widely accepted practice [1]–[4]. To our knowledge, Wanwan *et al* is the first to report the theoretical and experimental findings on the effect of Cd-diffusion thermal annealing on the resistivity of CdZnTe crystals (9). Based on this study, the average values of Cd self-diffusion coefficients of Cd_{0.9}Zn_{0.1}Te crystal annealed at 1073, 973, and 873 K are found to be 1.464×10^{-10} , 1.085×10^{-11} , and 4.167×10^{-13} cm²/s. Recently, Fochuk *et al.* reported a promising result on elimination of Te inclusion in CdZnTe crystals by short term thermal annealing under Cd, Zn, and Te-over pressure and the corresponding resistivity of the crystal for a range of annealing temperature [10].

II. EXPERIMENT

CdZnTe crystals with detector-grade quality grown by Northrop Grumman using the Bridgman furnace method were used. The crystals were cut approximately $5 \times 5 \times 5$ mm³. The surfaces of the CdZnTe slices used for the experiments were prepared by mechanical polishing, using a series of Al₂O₃ powders grades, decreasing in size from 5.0 to 0.1 microns as necessary. The material removed in this procedure (~ 200 μ m by mechanical polishing, ~100 μ m by etching) was sufficient to remove all surface damage caused by sawing the slices from the wafer. Next, the CdZnTe crystals were etched using a 2% Br-methanol solution.

In the experimental procedure, infrared images of the samples were taken before and after annealing. The samples are marked to track the locations and orientations of the Te inclusion being studied. Samples were annealed under Cd vapor overpressure and in vacuum at 600 °C for 45 minutes at a temperature gradient of 10 °C/cm. A second set CdZnTe post-growth annealing experiments was carried for the following annealing parameters: 700 °C CdZnTe annealing temperature, Cadmium temperature at 650 °C, 30 minutes annealing time, and temperature gradient of 10 °C/cm.

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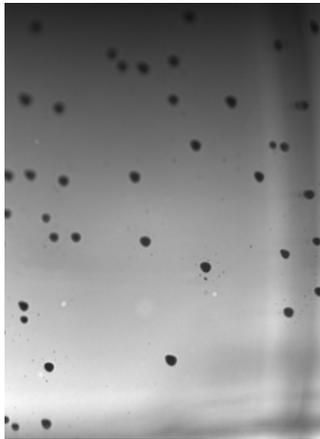
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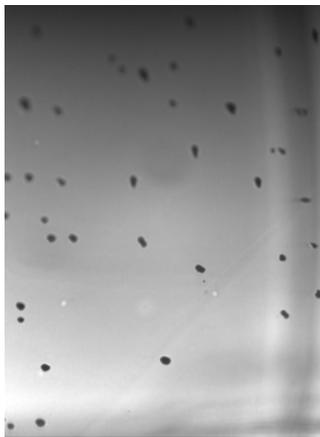
III. RESULTS

Figure 1 shows the infrared images of the same region of a CdZnTe crystal before annealing and for the first and second annealing cycles (at 600 °C, 45 minutes and temperature gradient of 10 °C/cm for each cycle).

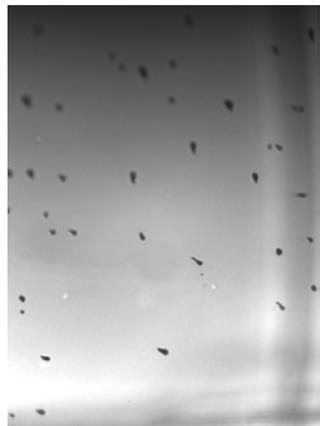
Low temperature side High temperature side



(a) Before annealing



(b) First annealing at 600 °C for 45 minutes



(c) Second annealing at 600 °C for 45 minutes

Fig. 1. Infrared images comparing Te inclusions sizes and locations of the same region in the CdZnTe crystal before annealing, and for the first and second annealing cycles (at 600 °C for 45 minutes for each cycle).

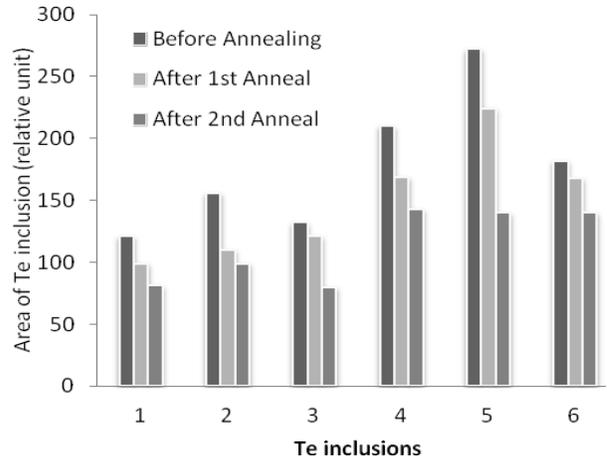


Fig. 2. Comparison of size reductions for six selected Te inclusions in the two annealing cycles. The areas were calculated using NIS-Elements Nikon imaging software.

In each annealing cycle, there are reductions in the sizes of the Te inclusions as indicated by the infrared images in Fig. 1. In addition to size reduction (see Fig. 2), the Te inclusions also migrate towards the high-temperature side of the sample. The migration of Te inclusions is clearly shown in Fig. 3 for the following annealing parameters: 700 °C CdZnTe annealing temperature, Cadmium temperature at 650 °C, 30 minutes annealing time, and temperature gradient of 10 °C/cm.

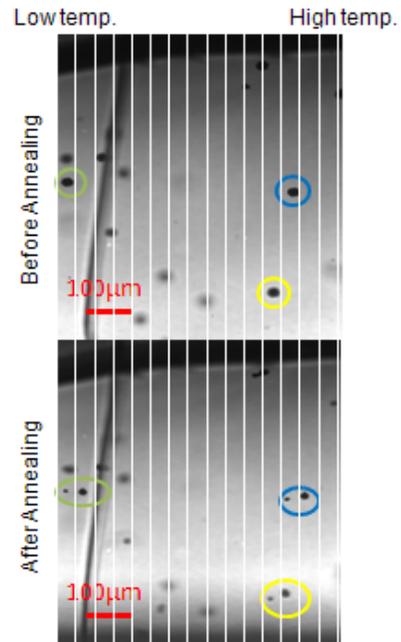


Fig. 3. Migration of Te inclusions towards the high-temperature in thermal gradient post-growth annealing of a CdZnTe crystal under Cd vapor overpressure.

Figure 2 shows the comparison of the size reductions for six selected Te inclusions in the two annealing cycles shown in Fig 1, with the areas calculated using NIS-Elements Nikon imaging software. The percentage reductions are shown in

Table I. Figures 1 and 3 show that for most of the Te inclusions, an inclusion separates into two with the larger portion migrating towards the high-temperature side of the sample, leaving the smaller portion behind.

TABLE I. PERCENTAGE REDUCTION OF TE INCLUSIONS

Te inclusion	Size before annealing	Reduction after first annealing	Reduction after second annealing
1	121	18%	18%
2	156	29%	10%
3	132	8%	34%
4	210	20%	15%
5	272	18%	38%
5	182	8%	17%

IV. CONCLUSION

Our studies have shown that annealing CdZnTe crystals under Cd vapor overpressure and in vacuum at 600 °C for 45 minutes at a temperature gradient of 10 °C/cm showed significant reduction in the size of Te inclusions. The reduction in sizes ranges from 8% to 38%. In addition, for most of the Te inclusions, an inclusion separates into two with the larger portion migrating towards the high-temperature side of the sample, leaving the smaller portion behind.

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