Contract No:

This document was prepared in conjunction with work accomplished under Contract No. 89303321CEM000080 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

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SRNL-STI-2021-00399

Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

Optimization of CZTS Gamma-Ray Detectors

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INMM-ESARDA Annual Meeting 2021

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8/25/2021 10:45:00 AM - 8/25/2021 12:30:00 PM

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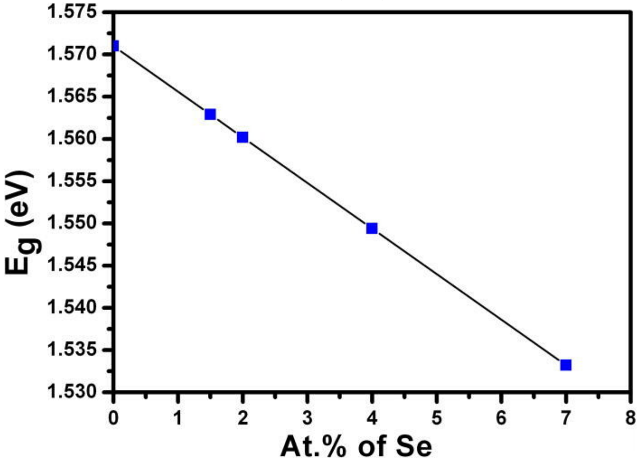
Optimization of CZTS Gamma-Ray Detectors: Selenium Concentration

- Some benefits of Se in CdZnTe matrix
  - Strong influence in modifying Zn segregation coefficient: better compositional homogeneity with increased Se concentration for THM grown ingots.
  - Effective solution hardening in arresting sub-grain boundaries and their network.
  - Decreased Te-inclusion/precipitate concentration.
- Factors to be considered for optimizing the CdZnTeSe composition
  - Retrograde solubility of tellurium with Zn concentration variation
  - Band-gap variation of the composition
  - Role of Se on carrier trapping for point defects, complexes and any extended defects

1. **Higher Zn concentration: higher concentration of Te inclusions/precipitates.**
2. **Higher Zn concentration: higher alloy broadening.**

Band-gap variation of $Cd_{0.9}Zn_{0.1}Te_{1-y}Se_y$

Band-gap of $Cd_{0.9}Zn_{0.1}Te_{1-y}Se_y$ vs. selenium concentration.



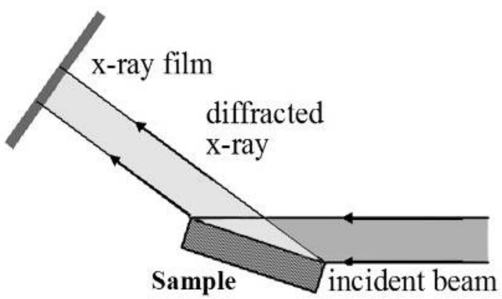
As the band-gap in CZTS decreases with increased selenium concentration, there is a tradeoff in finding the minimum amount of selenium compound for acceptable resistivity and the optimum CZTS composition for the lowest performance limiting defects.

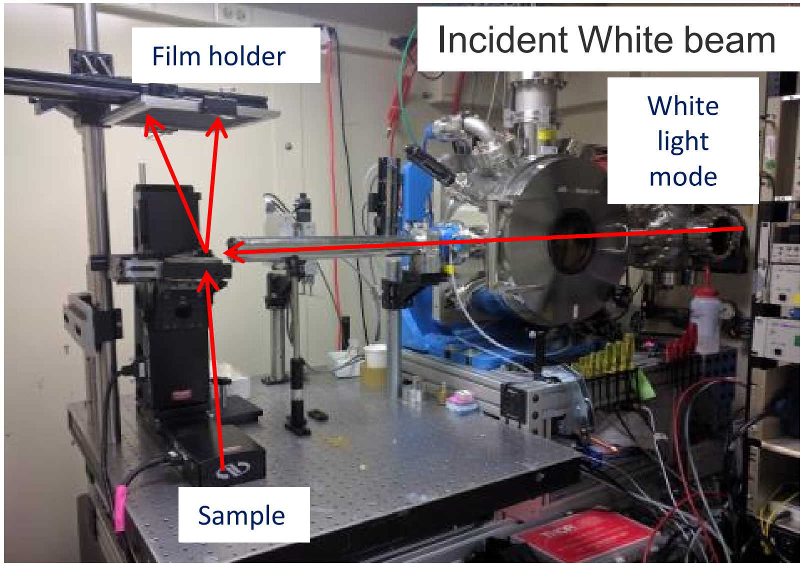
IR and LBNL ALS BL332 White Beam X-Ray Diffraction Topography (WBXDT)

Two techniques are being used to evaluate the presence of residual stress in CZTS:

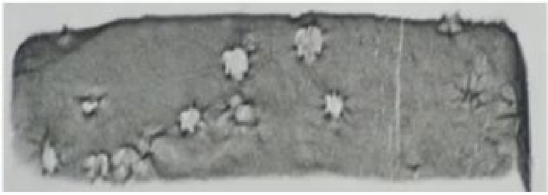
- IR transmission under crossed polarizers: Stress-induced birefringence causes localized transmission of light through the sample.
- WBXDT: Topographic image reveals structural deformation due to stress induced lattice-distortion.

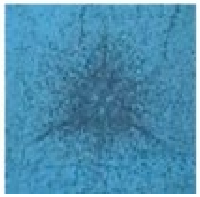
Reflection geometry

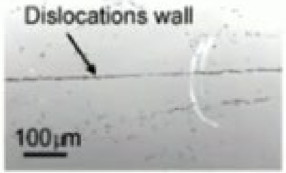




WXRD images



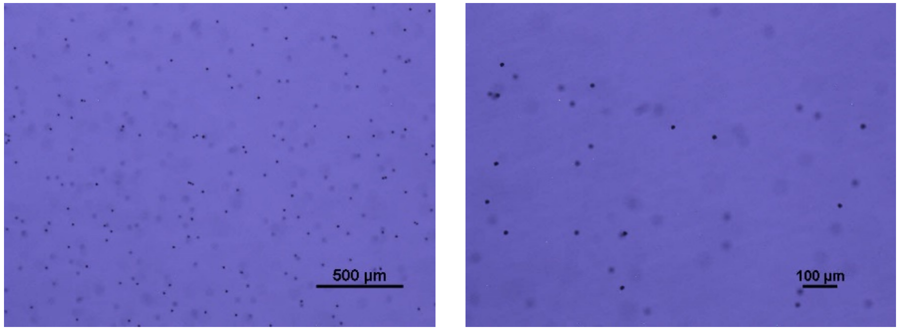




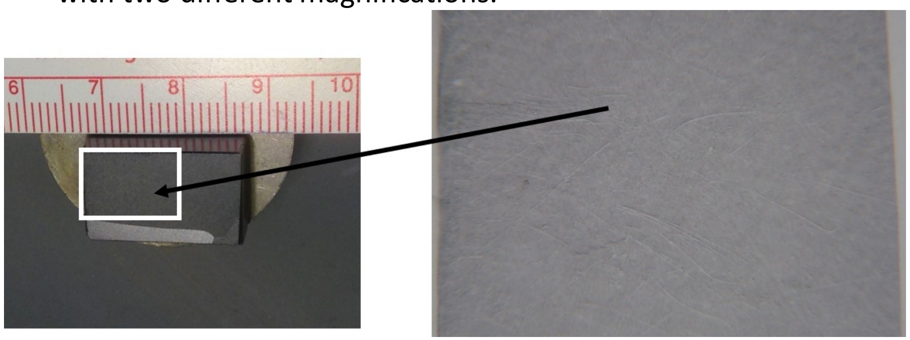
Residual thermal stresses are responsible for a non-uniform electric field distribution and sub-grain boundaries. A uniform electric field is critically important to attain high performing radiation detectors. Thus, avoidance and/or mitigation of high thermal stress in the materials is a strict requirement for enhanced detector performance.

X-ray topography and IR transmission image of THM-grown $Cd_{0.9}Zn_{0.1}Te_{0.985}Se_{0.015}$

$Cd_{0.9}Zn_{0.1}Te_{0.985}Se_{0.015}$



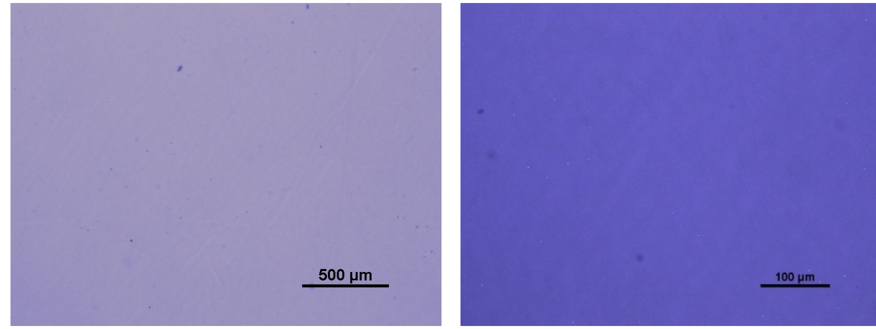
High-magnification IR transmission microscopic images with two different magnifications.



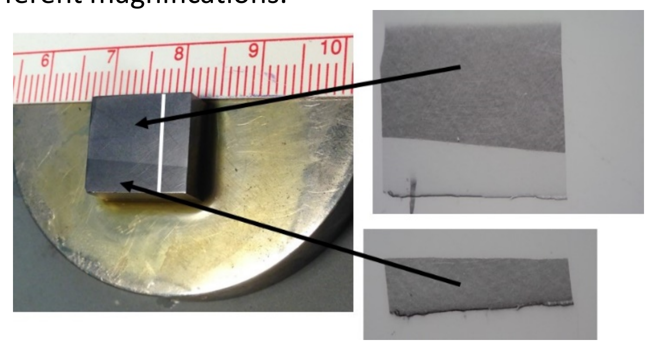
Optical photograph and the corresponding X-ray topographic image of a $Cd_{0.9}Zn_{0.1}Te_{0.985}Se_{0.015}$ sample.

The concentration and size of Te inclusions are comparable to as-grown CZT for CZTS with 1.5 atomic% of selenium. Thus. 1.5 atomic % of selenium composition is discarded, although the material is free from sub-grain boundary network.

$Cd_{0.9}Zn_{0.1}Te_{0.98}Se_{0.02}$



High-magnification IR transmission microscopic images with two different magnifications.

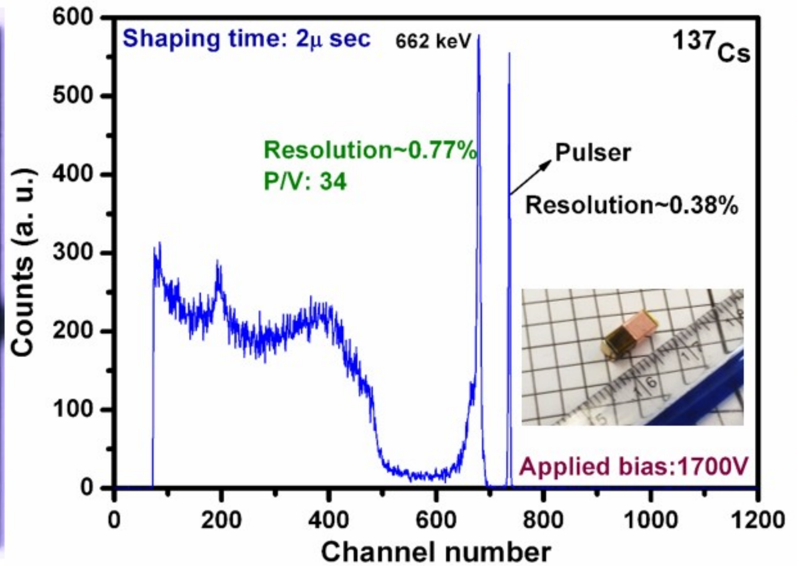


Optical photograph and the corresponding X-ray topographic image of a $Cd_{0.9}Zn_{0.1}Te_{0.98}Se_{0.02}$ sample.

The as-grown CZTS with 2 atomic% of selenium contains very low concentrations of Te inclusions. Additionally, the material is free from a sub-grain boundary network.

Apparently $Cd_{0.9}Zn_{0.1}Te_{0.98}Se_{0.02}$ is the optimum composition with highly reduced performance limiting defects among the different compositions used in this study.

Efficacy of Se addition in CZT matrix



As measured pulse height spectrum for a ^{137}Cs source of a Frisch-grid detector fabricated from as-grown $Cd_{0.9}Zn_{0.1}Te_{0.98}Se_{0.02}$ THM ingot. Left: IR transmitted image of the whole detector and right: X-ray topographic image of the whole detector. The inset shows the image of the fabricated detector.

Detector dimensions: $3.5x3.5x9.15\ mm^3$.

Efficacy of Se addition in CZT matrix

- Enhanced compositional uniformity (about 90% of the ingot length)
- About 1.5 times increase of hardness as compared to CZT
- Reduced thermal stress
- Drastic reduction of Te inclusions
- Substantial reduction of sub-grain boundary and free from sub-grain network

Charge Transport Properties of THM-grown CZTS with optimum 2% Se

Resistivity: $1\text{-}3x10^{10}\ \Omega$-cm

$\mu\tau_e$: $4.5\text{-}5\ x10^{-3}\ cm^2/V$ (average), $6.6x10^{-3}\ cm^2/V$ (highest)

Detector performance: Energy resolution is 0.9-1.1 % at 662 keV,

(~1-cm long Frisch grid detectors) best resolution achieved: ~0.77 % at 662 keV.

The composition with 2% Se ($Cd_{0.9}Zn_{0.1}Te_{0.98}Se_{0.02}$) was found to be *the best in terms of material properties and charge transport characteristics.*

We expect to improve the energy resolution (as measured) at 662 keV to between 0.5-0.6 % for THM-grown $Cd_{0.9}Zn_{0.1}Te_{0.98}Se_{0.02}$ by using purified starting material.

Thank you for your kind attention !