The U.S. Workshop on the Physics and Chemistry of II-VI Materials
Baltimore, Maryland, October 21-23, 2014

BNL-106296-2014-CP

Interfacial defects and elemental composition of chemically treated CdZnTe crystals

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October 23, 2014

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Introduction

- Surface processing plays an important role in controlling many aspects of device operation and is critical for assuring good performance;

- An imperfect surface of a substrate acts as a pathway for the movement of defects. Also acts as a source of trapping centers that distort the pulse height and enhances the surface leakage current in radiation detectors;

- Mechanical polishing followed by chemical etching is the commonly used method to produce non-conductive smooth surfaces for efficient charge transport and low leakage current;

- Chemical polishing, especially bromine-based solutions, induces a Te-rich surface and forms new chemical species on the surface.

Sample Preparation and Etching Process

➢ Samples: Methods for growth

CdZnTe: THM and Floating Zone (FZ)

➢ Crystal processing

- **Silicon Carbide abrasive papers and alumina powder with decreasing particle size, and a final polishing with 0.1-µm alumina powder against a multi-tex soft pad;**
- **Chemo-mechanical polishing with bromine-methanol solution and ethylene glycol.**

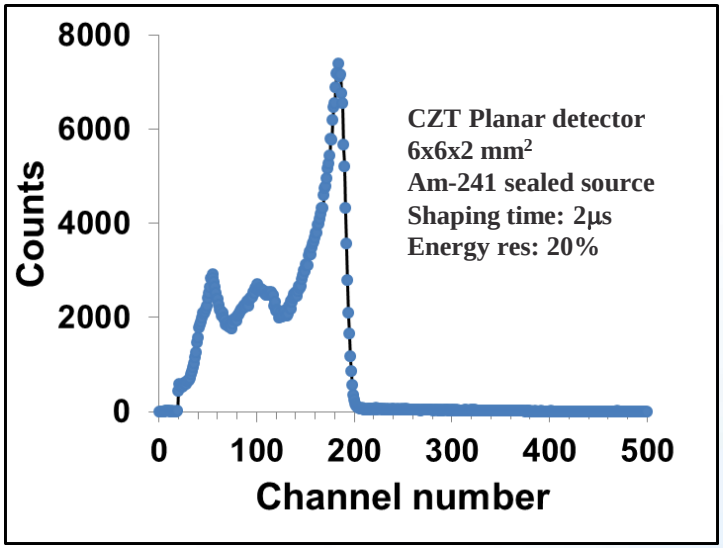
➢ Chemical etching for revealing EPDs

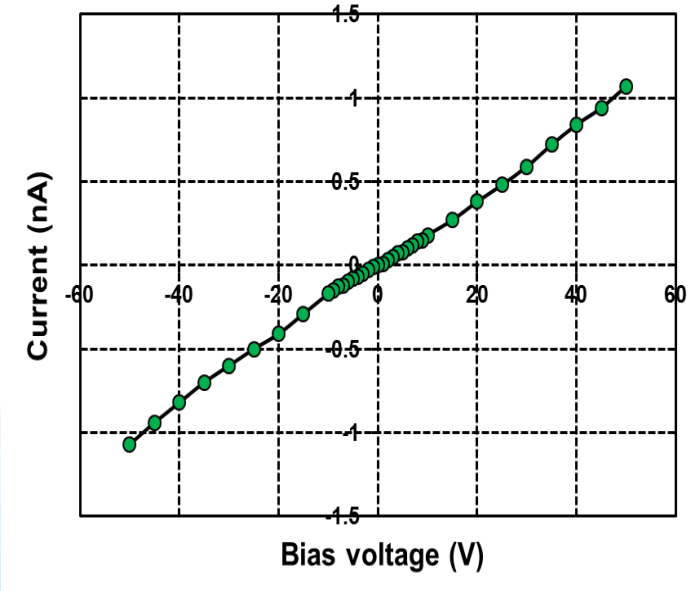
HF-based solutions were used to show dislocation-related etch pits.

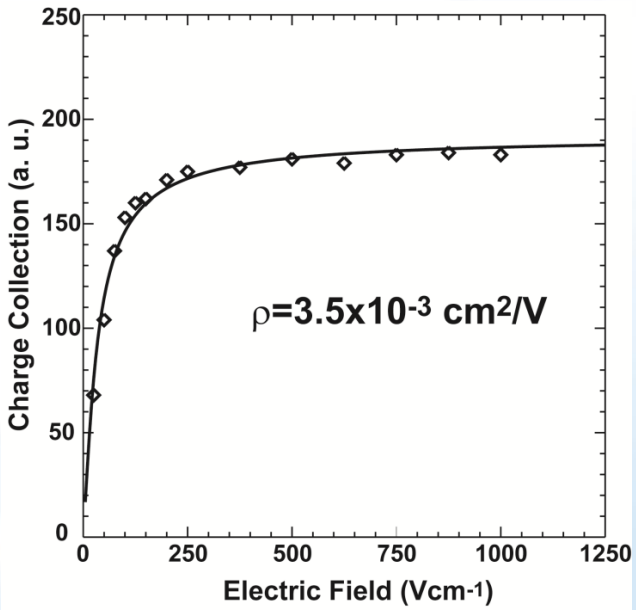
Etch pits were revealed on the crystallographic surfaces (111)A and (111)B.

Samples' Properties

HPB-grown CZT detector-grade crystals
Resistivity: $5x10^{10}$ Ω-cm
Mobility-lifetime product: $3.5x10^{-3}$ cm^2/V
Energy resolution: 20% for 59.5-keV gamma peak

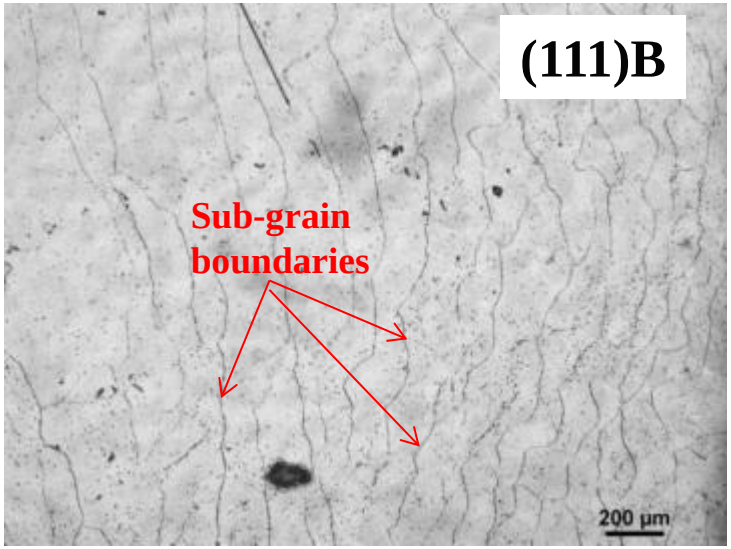




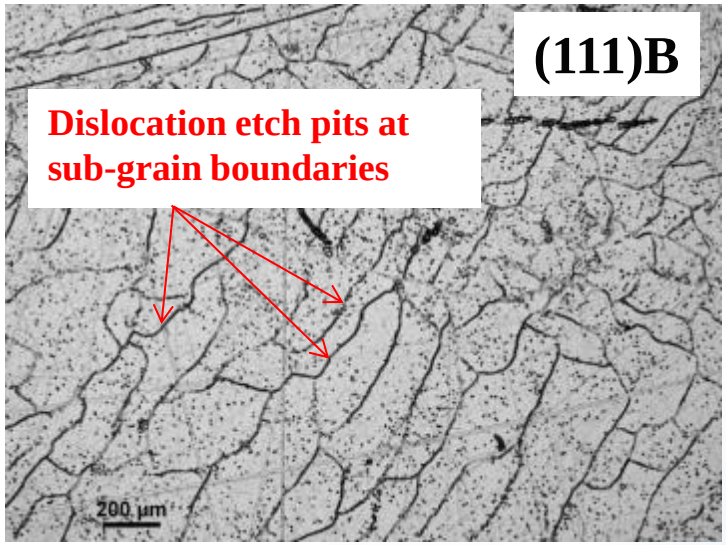


Defect Characterization

Grown-in Dislocations and Sub-Grain Boundaries



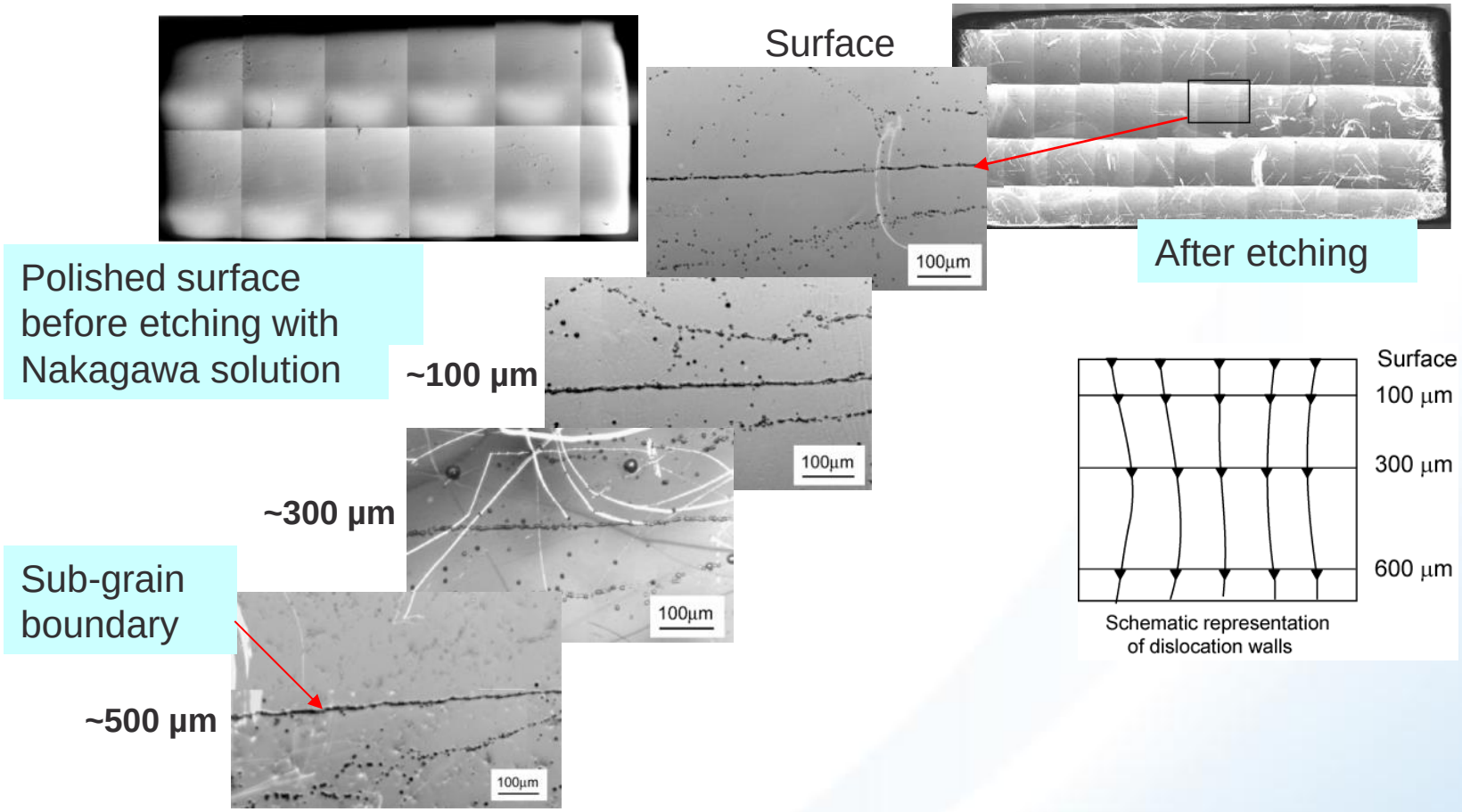
CZT crystal grown by the FZ method



CZT crystal grown by the THM method

- Dislocation etch pits align along the sub-grain boundaries;
- High concentration of etch pits clustered as cellular structure;
- High density of saucer pits formed around the indentation due to deformation dislocations

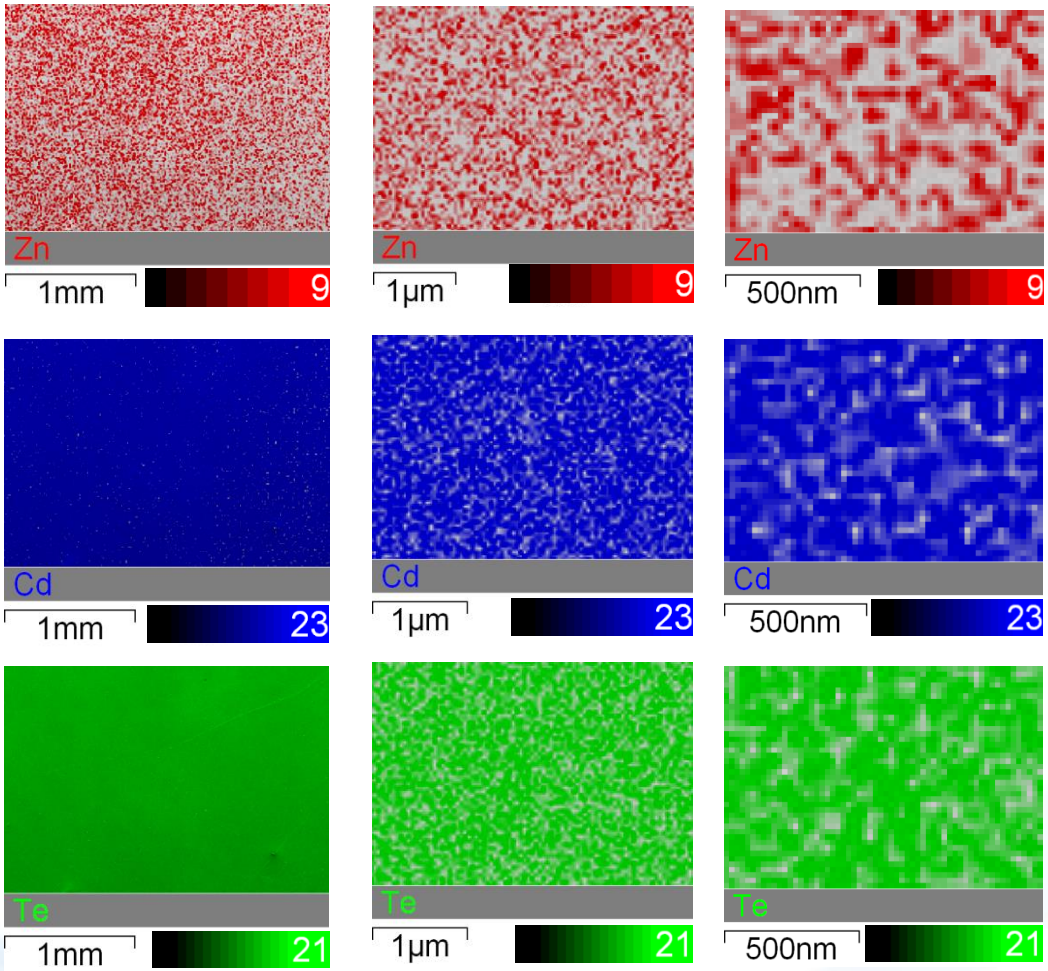
Dislocation Walls Extend in the Bulk



Such dislocations are caused by thermo-mechanical stresses during cooling or post-growth annealing. Very often, such walls go across the entire crystal thickness.

A. Hossain et al., J. Cryst. Growth, 310, 21 (2008) 4493–4498

Elemental Non-Uniformity in Large CZT Crystal



Images of elemental maps of a CZT crystal by electron dispersive spectroscopy with high intensity electron beam.

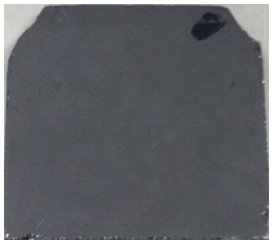
Non-homogeneous elemental distribution was revealed in nano-scale mapping.

Qualitative Distribution of Elemental Composition

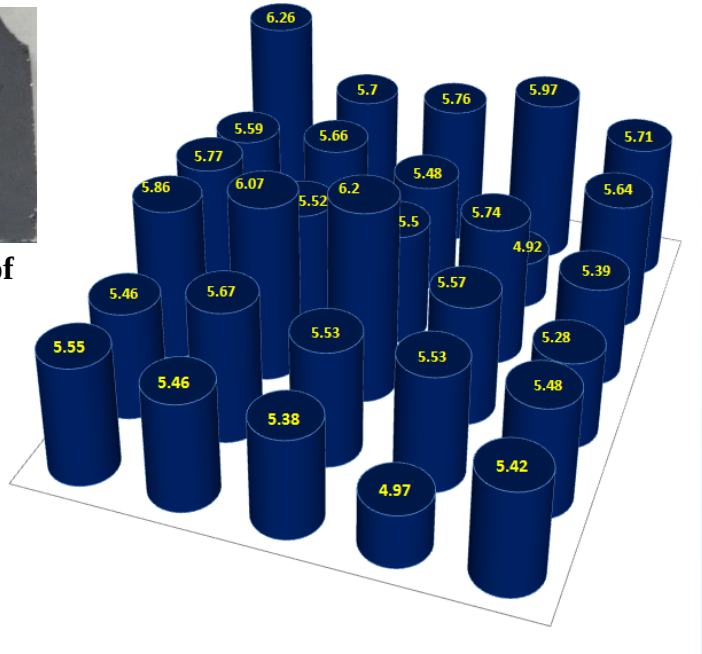
Spectrum processing:

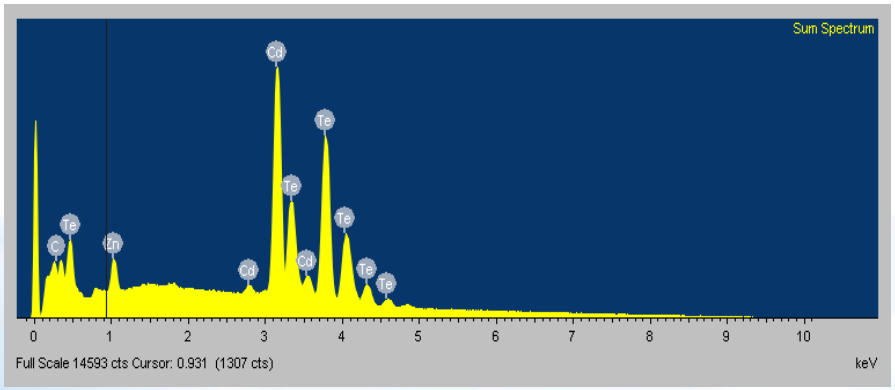
Processing option: All elements analyzed (Normalised)

Element	Weight%	Atomic%
Zn L	2.83	5.09
Cd L	43.63	45.61
Te L	53.54	49.30
Totals	100.00	



Optical image of CZT crystal

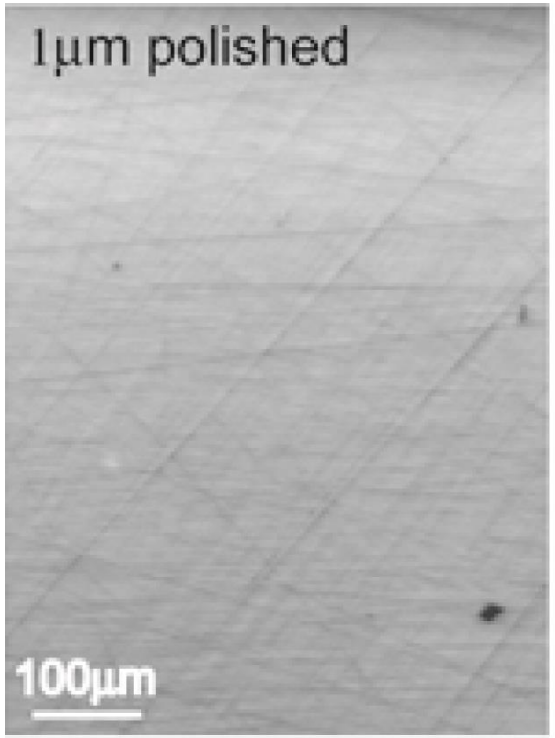




A quantitative mapping of Zn concentration (Atomic %) over the crystal's surface area. Zn variation within the 4 cm^2 area: 4.92 -6.26 (9.8% - 12.52)

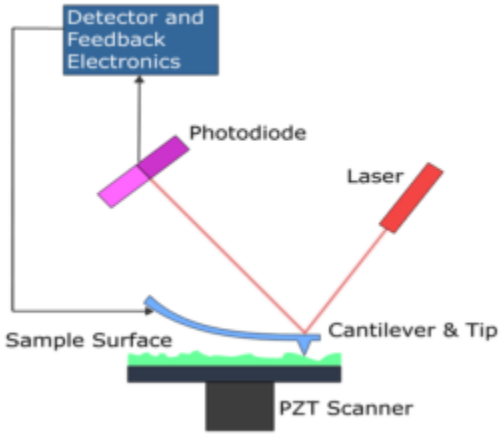
Surface Processing

Optical Images of Processed Surfaces



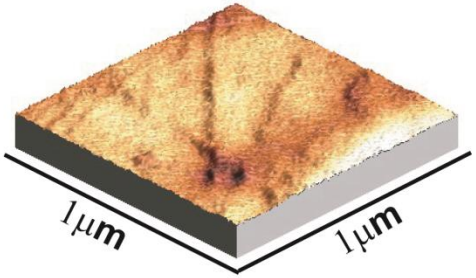
- Mechanical polishing generates scratches on the surfaces.
- Chemo-mechanical polishing (CMP) etches off scratches and leaves smoother surfaces
- The degree of roughness cannot be determined from the IR images.

Measurement of Surface Roughness



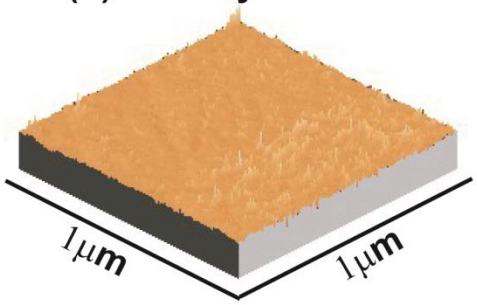
The degree of surface roughness assessed by AFM measurements.

(a) Mechanically Polished



RMS=5.12 nm
Avg. roughness=4.21nm
Peak-Peak = 37.1 nm

(b) CMP by B-M sol



RMS=0.72 nm
Avg. roughness= 0.66 nm
Peak-Peak = 15.9 nm

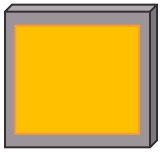
Processed surfaces were evaluated by Atomic Force Microscopy (AFM).

AFM tapping mode
Resonance frequency ~ 250 kHz
Scanning speed 1-2 Hz

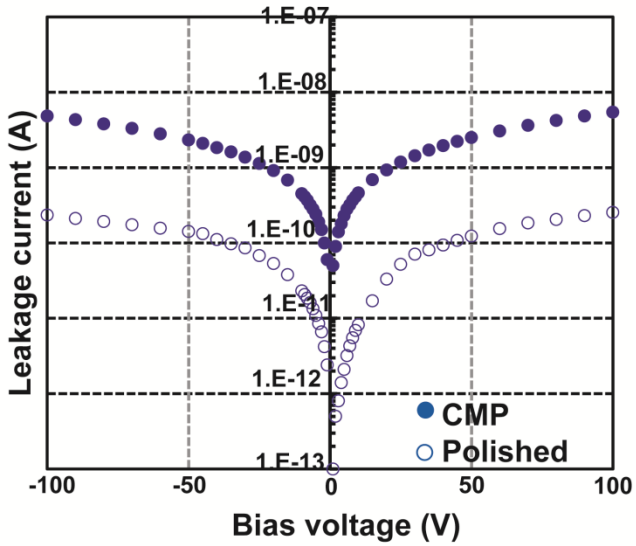
- **Mechanical polishing damage appears on fig. (a).**
- **BM etching removes damage, but some planarity issue remains.**

XPS Peaks of Chemically Polished Surfaces

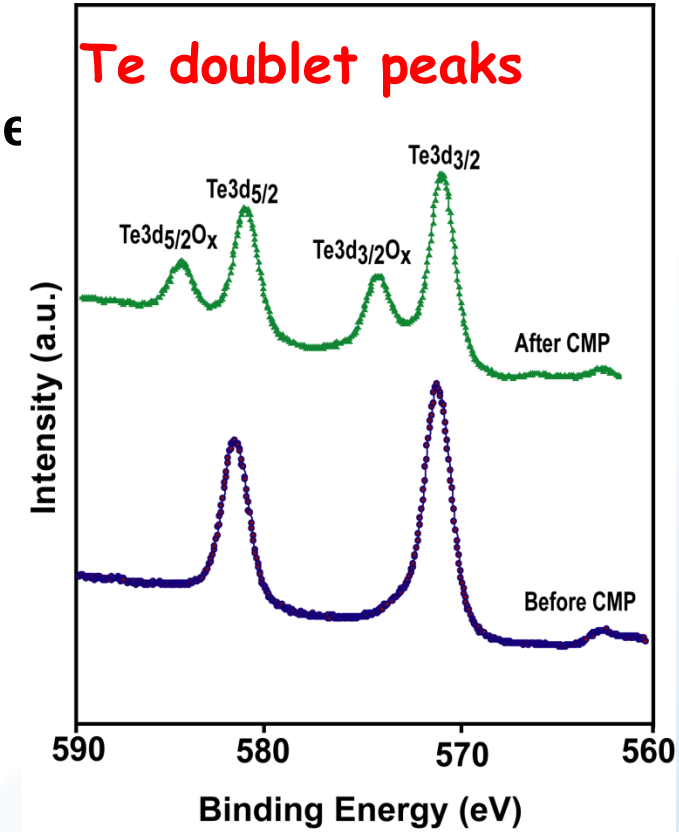
Bromine-based solution yields a Te-rich surface that oxidizes in air over time and causes an increase in the surface leakage current.



Au-CZT-Au Planar detector

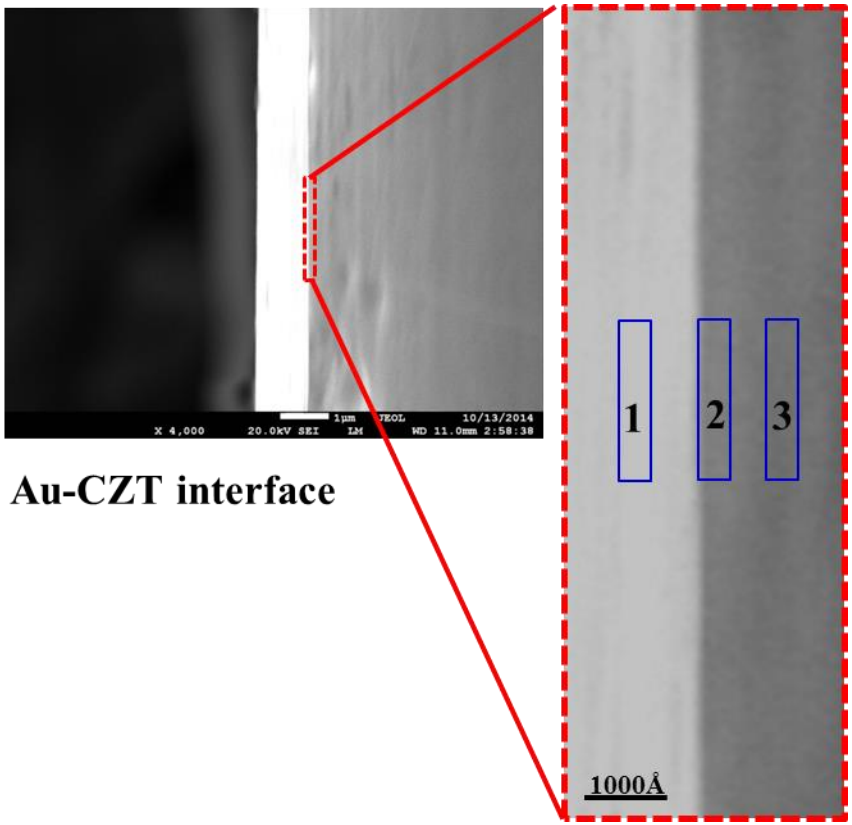


Leakage current increased an order of magnitude after CMP

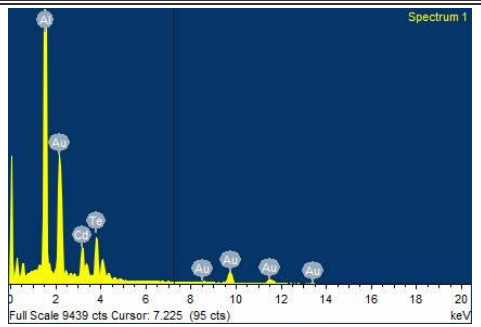


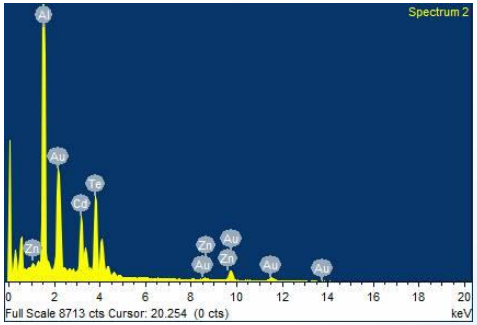
Formed TeO_X after oxidation in air, which shifts the peak to higher binding energy.

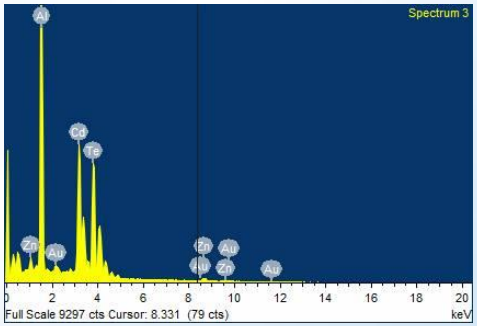
Metal-Semiconductor Interface



Au-CZT interface





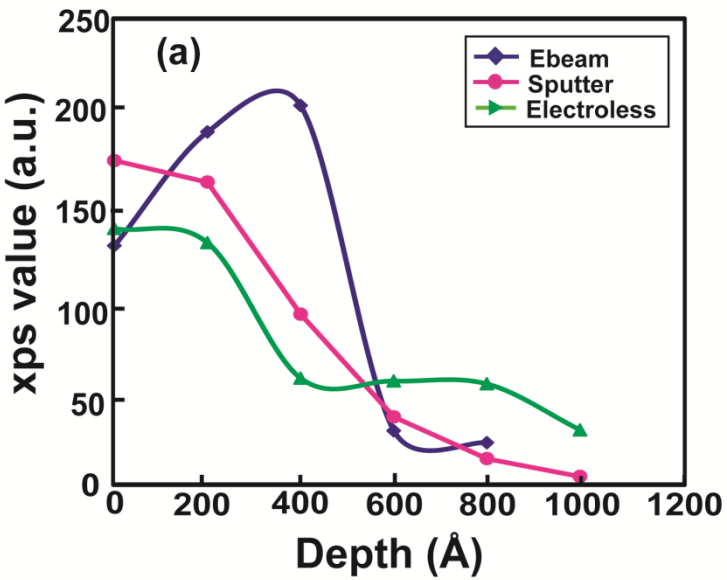


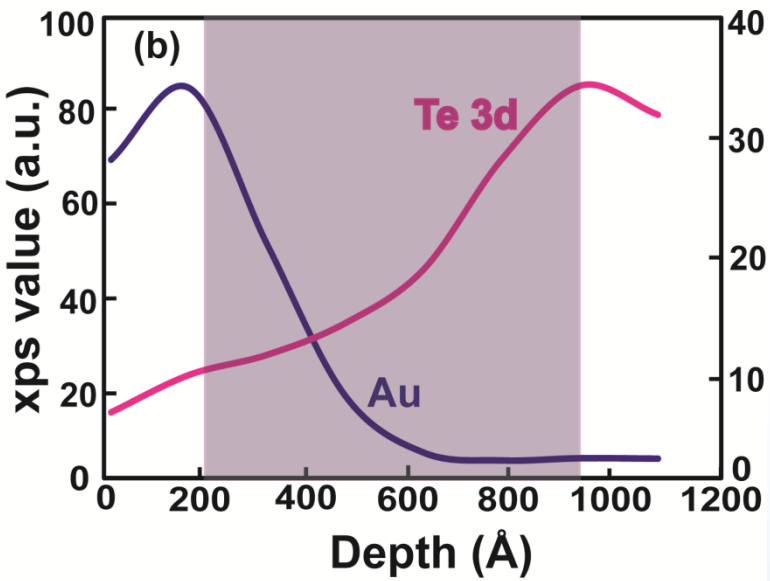
Achieved smooth interface by optimizing the surface process and metal deposition technique.

EDS spectra display that Au is diffused into the bulk.

Spectra of EDS measurement around the Au-CZT interface

Diffusion Profile of Metals at Interface





Au diffusion pattern at Au-CZT interface.

Interface layer was about 600Å wide.

Au was deposited on identically processed surfaces using electron beam, sputter and electroless methods.

- Diffusion of Au into CZT was found to be lower for electron beam deposition compared to other methods.
- Electroless method seems to generate strong and uniform bonding of Au and CZT.

Summary

- Demonstrated various bulk defects (e.g., dislocations and sub-grain boundaries) and surface defects, and examined their effects on the performance of devices;
- Bromine-based solution yields Te-rich surface that easily oxidized to form a native oxide and increased the leakage current;
- Optimized the processing technique to increase the surface planarity, reduce the concentration of nano-scale defects at the surface, and increase the device stability over time;
- Achieved flat interface by optimizing the surface processing technique and metal deposition method.

Acknowledgement

This work was supported by U.S. Department of Energy, Defense Nuclear Nonproliferation Research and Development, DNN R&D.

~:Thank you:~

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