Contract No:

This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-08SR22470 with the U.S. Department of Energy (DOE) Office of Environmental Management (EM).

Disclaimer:

This work was prepared under an agreement with and funded by the U.S. Government. Neither the U.S. Government or its employees, nor any of its contractors, subcontractors or their employees, makes any express or implied:

- 1) warranty or assumes any legal liability for the accuracy, completeness, or for the use or results of such use of any information, product, or process disclosed; or
- 2) representation that such use or results of such use would not infringe privately owned rights; or
- 3) endorsement or recommendation of any specifically identified commercial product, process, or service.

Any views and opinions of authors expressed in this work do not necessarily state or reflect those of the United States Government, or its contractors, or subcontractors.

SRNL-STI-2020-00512 **Surface Composition Studies of** CdZnTe Material Using X-Ray **Photoelectron Spectroscopy**

Mebougna L. Drabo,¹ Alexander A. Egarievwe,¹ Ezekiel O. Agbalagba,² Richard M. Lagle,¹ Stephen U. Egarievwe,¹ Utpal N. Roy,^{3.4} and Ralph B. James⁴

¹Alabama A&M University, Nuclear Engineering and Radiological Science Center, Huntsville, Alabama, USA ²Federal University of Petroleum Resources, Physics Department, Effurun, Delta State, Nigeria ³Brookhaven National Laboratory, Nonproliferation and National Security, Upton, New York, USA ⁴Savannah River National Laboratory, Science and Technology, Aiken, South Carolina, USA

U.S. Department of Energy/NNSA, Office of Defense Nuclear Nonproliferation Research and Development



FUNDING SOURCES

National Science Foundation (NSF) MRI Award 1726901 and NSF HBCU-UP TIP Award 1818732

November 4-6, 2020







Savannah River

lational Laboratory





Outline

- Introduction
- Experiments and Methods
- High-Performance XPS Surface Analysis System
- XPS Data Collection
- Results
- Summary and Conclusion





Introduction

- Cadmium zinc telluride (CdZnTe or CZT) is widely used for the detection of X-rays and gamma rays at room-temperature without cryogenic cooling.
- It has many applications in the areas of nuclear and radiological threat detection, medical imaging, gamma spectroscopy, and astrophysics.
- The composition of the detector wafer surfaces is a very important factor in detector device fabrication.
- The stoichiometric composition of the detector surfaces affects its surface current which in turn contributes to the electronic noise.
 - High electronic noise is detrimental to the energy resolution of the detector device.
- The mechanical stability at the interface of the electrical contacts and the detector material is an important factor in terms of durability and shelf-life of detector devices.



Experiments and Methods – Sample Preparation

- CdZnTe sample of size 6.4 x 6.9 x 2.4 mm³ was cut using a machine equipped with a diamond impregnated wire saw.
- After cutting, the sample was mechanically polished on a silicon carbide abrasive paper using distilled water.
 - Large grain of 800-grit paper was first used, followed by polishing on 1200-grit paper.
- The wafer was further polished on a MultiTex paper using alumina power and distilled water to get mirror-shine surfaces.
 - A 3.0-µm alumina powder was first used.

CHAMPIONING Change Education

20 AffWIAE and IAJC Virtual Joint Conference

November 4-6, 2020

- This is followed with successive polishing in decreasing sizes of powder down to 0.1 μm.
- A separate MultiTex pad was used for each alumina powder size.
- After each polishing, the sample is thoroughly rinsed in distilled water.



High-Performance XPS Surface Analysis System

CHAMPIONING Change Education

O ATMAE and IAJC Virtual Joint Conference

November 4-6, 2020



Figure 1. High-performance XPS Surface Analysis System by Thermo Fisher.



Experiments and Methods – XPS Data Collection

- The CdZnTe wafer was mounted on a sample holder and loaded to the XPS machine.
 - The XPS machine is equipped with an X-ray source gun type AI-K-Alpha.
- A spot size of 400 µm was used on the sample.

CHAMPIONING Change Education

20 ATMAE and IAJC Virtual Joint Conference

November <mark>4-6, 202(</mark>

- The photoelectrons ejected from the sample surface are collected in the analyzer.
- A survey analysis was first made to scan for all elements that could be present on the surface.
 - In the survey scan, the analyzer mode was set at a pass energy of 200.0 eV, and the energy step size was 1.00 eV. The scan took 68 seconds.
- Scans were made for specific energy regions of the dominant surface species.
 - The specific elements of interest studies in this experiment include Zn, Cd, and Te.
 - The analyzer mode for these scans was set at a pass energy of 50.0 eV, and the energy step size was 0.100 eV.



Results





Te3d



Figure 2. XPS survey scan showing the presence of Zn, Te, O, Cd, C, Cl, and Si.





Cadmium Peaks



Figure 3. XPS scan showing the $Cd3d_{5/2}$ and $Cd3d_{3/2}$ peaks of cadmium.





Zinc Peaks



Figure 4. XPS scan showing the $Zn2p_{5/2}$ and $Zn2p_{3/2}$ peaks of zinc.



Tellurium and Tellurium Oxide Peaks

CHAMPIONING Change Education

O ATMAE and IAJC Virtual Joint Conference

November 4-6, 2020



- The XPS scan for Te also showed TeO₂ peaks.
- This is an indication of the formation of TeO₂ on the surfaces of the CdZnTe wafers.





Tellurium and Tellurium Oxide Peaks

CHAMPIONING Change Education

O ATMAE and TAJC Virtual Joint Conference

November 4-6, 2020

Table 1. Heights of the binding energy peaks identified for Cd, Zn, Te, and TeO₂.

Peak	Binding Energy (eV)	Peak Height Raw Counts
Cd3d _{5/2}	405.08	323697
Cd3d _{3/2}	411.78	245079
Zn2p _{3/2}	1021.58	200017
Zn2p _{1/2}	1044.98	190753
Te3d _{5/2}	572.78	178127
Te3d _{5/2} O ₂	575.08	451401
Te3d _{3/2}	583.18	174938
Te3d _{3/2} O ₂	586.38	376005



Summary and Conclusion

CHAMPIONING Change Education

90 ATMAE and IAJC Virtual Joint Conference

November 4-6, 2020

- We have used XPS to determine the dominant elements on CdZnTe wafer surface.
- The XPS results showed the presence of Zn, Te, O, Cd, C, Cl, and Si, and TeO₂.
- The XPS scans focused on the binding energies in the regions of Cd, Zn, and Te showed that these elements are significantly present as expected.
- The XPS scan for Te also showed TeO₂ peaks.
 - This is an indication of the formation of TeO_2 on the surfaces of the CdZnTe wafers.
- In future studies, we plan to investigate the near-surface compositional variation by using high-speed ions to remove very thin surface layers of the CdZnTe wafer

THANK YOU