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Surface Composition Studies of CdZnTe Material Using X-Ray Photoelectron Spectroscopy

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Abstract

High-resistivity zinc cadmium telluride (CdZnTe) semiconductor is a very popular material for room-temperature nuclear detection applications. It is used for the detection of X-rays and gamma rays in many areas: nuclear and radiological threat detection, medical imaging, gamma spectroscopy, and astrophysics. Mechanical stability at the interface of electrical contacts and the detector material is an important factor in terms of durability and shelf life of detector devices. Other engineering factors where that interface plays an important role include thermal expansion due to temperature changes and vibrations that may result from certain applications. The surface composition of the material play an important role in the surface stability of the material. The stoichiometric composition of the detector surfaces also affects its surface current, which, in turn, contributes to electronic noise. High electronic noise is detrimental to the energy resolution of the detector device. X-ray photoelectron spectroscopy (XPS) is a good technique for determining dominant surface composition of materials. In this current study, the authors used an XPS to look at the dominant composition materials on the surface of a CdZnTe wafer. The experiments involved loading CdZnTe wafers into the XPS machine and recording the peaks of the binding energies of elements and compounds present on the surfaces. The XPS results showed the presence of Zn, Te, O, Cd, C, Cl, Si, and TeO_2. These results are important in the engineering of CdZnTe radiation detection devices.

Introduction

Zinc cadmium telluride (CdZnTe) is one of the most widely used materials 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 (James, Schlesinger, Lund, & Schieber, 1995; Zhang, Zhang, Lu, Yang, & Ren, 2013; Barber, 1999; Verger et al., 2001). The composition of the detector wafer surfaces is a very important factor in detector device fabrication (Egarievwe, Lukosi, Okwechime, Gul, Hossain, & James, 2016). It is important to have very low surface current to reduce noise in the detector signal. In the study of CdZnTe wafers that were etched in a solution of hydrogen bromide, hydrogen peroxide, and ethylene glycol, XPS measurements were used to quantify the formation of TeO_2 on the surfaces (Egarievwe, Lukosi, Okwechime, Gul, Hossain, & James, 2017). The authors found that the TeO_2 species that formed on the CdZnTe wafers immediately after etching contributed to an increase in the surface leakage current (Egarievwe et al., 2017).

The stoichiometric composition of the detector surfaces also affected its surface current, which, in turn, contributed 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. It is also important in thermal expansion, due to temperature changes and vibrations that may result from certain applications. The surface composition of the material plays an important role in the stability of the wafer surfaces, and in the engineering of CdZnTe nuclear detector devices. XPS has been used in several studies of CdZnTe materials, mostly for photodetection applications. When fabricating CdZnTe detector devices, the wafers are cut from large crystals. Afterwards, the wafers are polished to smooth their surfaces. The smoothing of the surfaces is often accomplished through two major successive processes of mechanical polishing and chemical etching (Egarievwe et al., 2019). Mechanical polishing involves using different grains of abrasive carbide papers, followed by alumina power and chemical etching, which involves dipping the wafer in a bromine methanol (Br -MeOH) solution (Egarievwe et al., 2019).

Chemo-mechanical is one of several recent methods for smoothing CdZnTe wafer surfaces, and XPS has been used to study the mechanical polishing, chemical etching, and chemo-mechanical polishing processes (Adams, Roy, Egarievwe, Agbalagba, Gul, Hossain, & James, 2019; Egarievwe, Hossain, Okwechime, Gul, & James, 2015; Sheahan, Martinez, Cooper, Mackenzie, Burgess, Kumar, & Furlong, 2019; Song et al., 2020). In a comparative study, XPS results showed that the chemical etching process resulted in the formation of more TeO_2 on CdZnTe detector surfaces compared to chemo-mechanical polishing (Adams et al., 2019). In the study of the two chemical solutions, XPS results showed that the tellurium oxide to tellurium binding-energy peak ratios for the mechanical polishing process were reduced by chemo-mechanical polishing using a bromine-methanol-ethylene-glycol solution compared

with hydrogen bromide in a mixture of hydrogen-peroxide and ethylene-glycol solution (Egarievwe et al., 2015). In a recent study, Song et al. (2020) used XPS to investigate the effects of inductively coupled Ar plasma etching (ICP-Ar) of CdZnTe wafers compared to Br-MeOH and found that the presence of TeO_2 on samples etched in Br-MeOH was absent on ICP-Ar etched samples. It was observed that the absence of the formation of TeO_2 on the ICP-Ar-etched CdZnTe detector resulted in a significant reduction of leakage current and an improvement of 12% in energy resolution (Song et al., 2020).

The deposition of electrical contacts is another important part of engineering CdZnTe nuclear detectors. The electrode (contact) material and the contact-wafer interface are important for the performance of the device. Ling et al. (2019) used XPS measurements to analyze the composition of different electrodes on CdZnTe detector surfaces. Gao, Sun, Yang, Wangyang, Zhang, and Zhu (2020) used XPS to effectively investigate the chemical composition of CdZnTe films that were grown by a hybrid method that combined two crystal growth techniques: physical vapor transport (PVT) and vacuum thermal evaporation (VTE) methods. XPS was also used to investigate the compositional disparity and surface lattice defects in CdZnTe films grown on aluminum nitride (AlN) ceramic substrates (Shen et al., 2019). The lattice defects were determined using the Te peak area ratio of CdZnTe to the total of the CdCnTe/AlN composite structure (Shen et al., 2019).

Experiments and Methods

X-ray photoelectron spectroscopy (XPS) is a good technique for determining dominant surface composition of materials. In this current study, an XPS was used to look at the dominant composition materials on CdZnTe wafers at and near the surface. The experiments involved loading CdZnTe wafers into the XPS machine and recording the peaks of the binding energies of elements and compounds present on the surfaces. The samples were analyzed using a high-performance XPS surface analysis system manufactured by Thermo Fisher and bought by Alabama A&M University with funding from the NSF-MRI support grant. It was equipped with software that could identify the binding energies of the surface species.

Prior to the XPS measurements, the CdZnTe sample—6.4 x 6.9 x 2.4 mm^3—was cut using a machine equipped with a diamond-impregnated miter saw. Water was used as a lubricant and coolant during the cutting process. After cutting, the sample was mechanically polished using a silicon carbide abrasive paper in distilled water. Large-grain, 800-grit paper was used first, followed by polishing on 1200-grit paper. The wafer was further polished with a MultiTex paper using alumina powder and distilled water in order to yield mirror-shine surfaces. A 3.0-µm alumina powder was used first, followed by successive polishing with 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 was thoroughly rinsed in distilled water. The sample was then chemically etched using a mixture of hydrogen bromide and hydrogen peroxide in an ethylene glycol solution.

The CdZnTe wafer was mounted on a sample holder and loaded into an XPS machine equipped with an X-ray source, gun-type Al-K-Alpha. A spot size of 400 µm was used on the sample. The photoelectrons ejected from the sample surface were collected in the analyzer. Figure 1 shows the survey analysis that was first made to scan for all elements that could be present on the surface. This was followed by looking at specific energy regions of the dominant species. 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. The specific elements of interest studied in this experiment included 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.

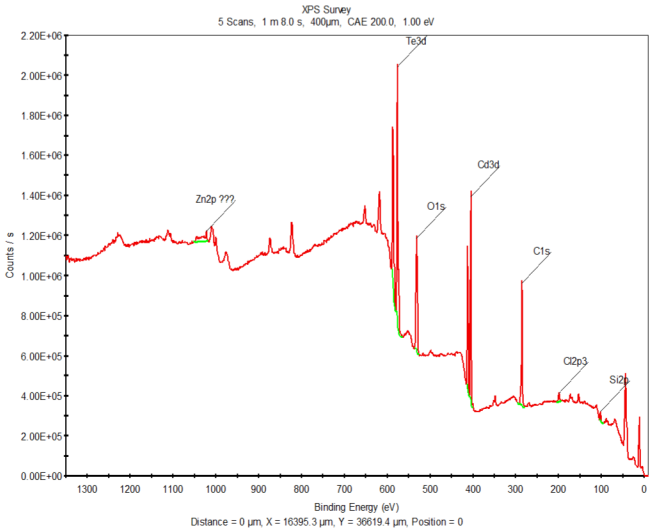

Figure 1. XPS survey scan showing the presence of Zn, Te, O, Cd, C, Cl, and Si.

Results and Discussion

Figure 1 shows the survey spectrum for the CdZnTe wafer, as recorded by the XPS system. It also shows the presence of zinc, tellurium, oxygen, cadmium, carbon, chlorin, and silicon. The survey scan was in the biding energy range of 0–1350 eV. Figures 2-4 shows the scans that focused on Cd, Zn, and Te, respectively. Figure 2 shows the $Cd3d_{5/2}$ and $Cd3d_{3/2}$ peaks at the binding energies of about 405.08 eV and 411.78 eV, respectively, corresponding to the elemental state of cadmium. The two peaks in Figure 3 correspond to $Zn2p_{3/2}$ and $Zn2p_{1/2}$ at 1021.58 eV and 1044.98 eV, respectively. Figure 4 shows the peaks for Te and TeO_2. This implies that there was some oxidation on the CdZnTe wafer. The $Te3d_{5/2}$ and $Te3d_{3/2}$ peaks were at bind-

ing energies of about 572.78 eV and 583.18 eV, respectively, corresponding to the elemental state of tellurium. The other two peaks were at approximately 575.08 eV and 586.38 eV, near the Te3d doublet peaks, and they show the formation of the TeO_2 species derived from the Te species present on the surfaces of the CdZnTe wafer. Table 1 summarizes the heights of the peaks.

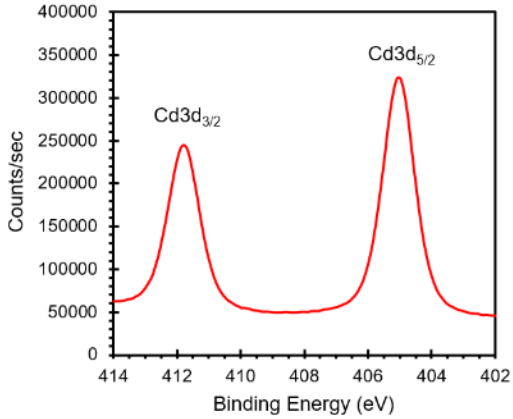

Figure 2. XPS scan showing the $Cd3d_{5/2}$ and $Cd3d_{3/2}$ peaks of cadmium.

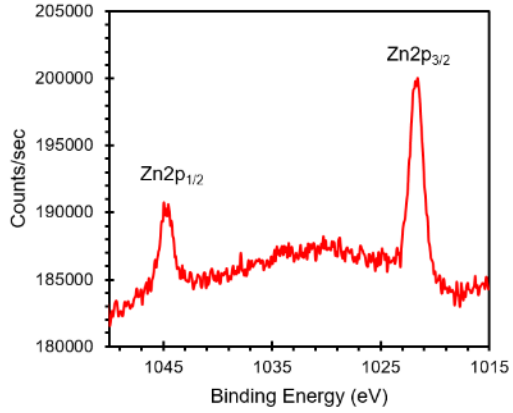

Figure 3. XPS scan showing the $Zn2p_{5/2}$ and $Zn2p_{3/2}$ peaks of zinc.

The XPS machine had the capability of using high-speed ions to remove very thin surface layers from samples. This enabled measurement and analysis of near-surface layers. Figure 5 shows the results of the measurements for a CdZnTe wafer before and after etching with high-speed ions. The data are from the same data sets used by Egarievwe, Lukosi, Okwechime, Gul, Hossain, and James (2020). As shown by the $Te3d_{5/2}O_2$ and $Te3d_{3/2}O_2$ peaks, the presence of TeO_2 that was observed before the etching was significantly reduced after etching. Unlike the wafer in Figure 4, this sample was not chemically etched using a mixture of hydrogen bromide in a hydrogen peroxide and ethylene glycol solution. Thus, the chemical etching resulted in the formation of significant amounts of TeO_2 on the surfaces of the wafer in Figure 4.

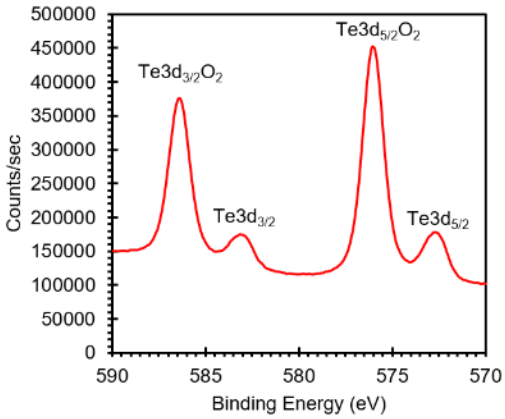

Figure 4. XPS scan showing the $Te3d_{5/2}$ and $Te3d_{3/2}$ peaks of tellurium and $Te3d_{5/2}O_2$ and $Te3d_{3/2}O_2$ peaks of TeO_2.

Table 1. Heights of the binding energy peaks identified for Cd, Zn, Te, and TeO_2.

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

Conclusions

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

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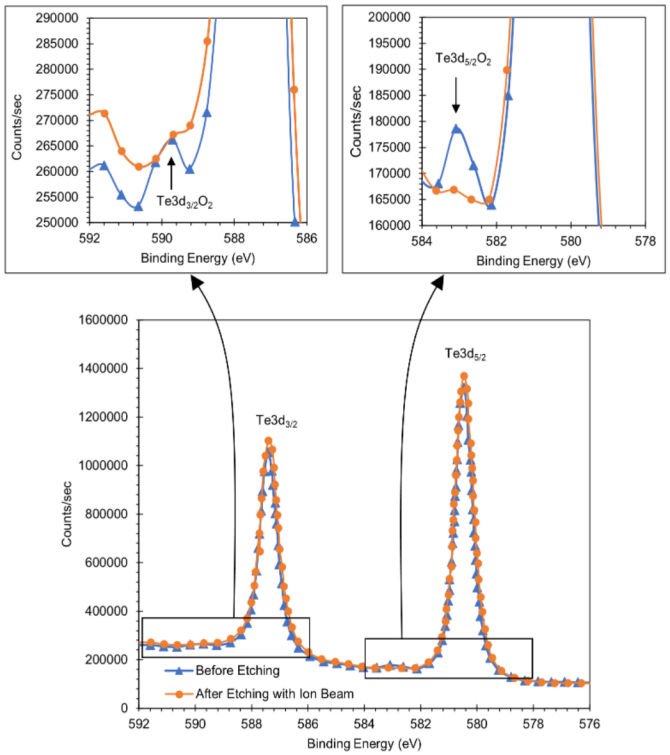

Figure 5. XPS scan showing the absence of $Te3d_{5/2}O_2$ and $Te3d_{3/2}O_2$ peaks after etching the CdZnTe wafer using high-speed ions. From the same datasets used by Egarievwe et al. (2020).

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