Fabrication and Photoelectron Spectroscopy of Sn-Based Intermetallic Compounds

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Abstract:

This paper explores the physical properties of tin-based intermetallic compounds AuSn, $AuSn_2$, and $AuSn_4$ for their potential application in sustainable energy. Using x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS), the study reveals how increasing the tin content alters their crystal structure and electronic properties leading to unexpected shifts in binding energy and work function values. These findings suggest the need for further research to explore the complexity of the system and optimize the material for future sustainable energy applications.

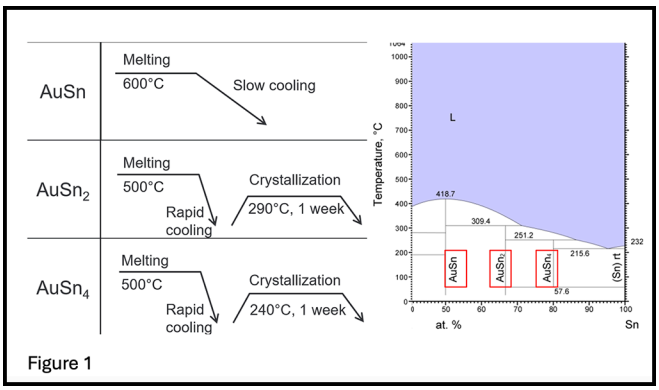


Figure 1

Introduction:

In a world that is continuing towards a decarbonized future, the pursuit of materials for sustainable eco-friendly energy solutions with tailored physical and chemical properties is crucial. Among these materials, tin-based intermetallic compounds, particularly AuSn, $AuSn_2$, and $AuSn_4$, have attracted attention recently in our group for their potential applications in various energy-related technologies. These intermetallic compounds have unique crystal structure and physical properties that alter with the amount of tin in the sample. Understanding how the material works and what is driving the physical changes is key in optimizing the performance of the future technology for practical applications.

One of the potential approaches for the materials exploration has been reported in the discovery of electrides. This is a class of materials with a unique crystal structure where the electrons serve as anions. These materials have been shown to exhibit unusual physical properties both electronically and optically. The study of these materials provides valuable insights into the relationship between the crystal structure and fundamental physical properties, possibly providing a solution for the interesting properties seen in the tin-based compounds.

This paper explores the unique physical properties seen with highly pure AuSn, $AuSn_2$ and $AuSn_4$. By examining the impact of the tin content in the compound through the XPS data and work functions, this study aims to shed light on the potential of these materials and the advancing development of eco-friendly energy technologies.

Materials and Methods. In creating the samples for analysis in the study, each compound was synthesized slightly differently. For the AuSn sample, the melting point was higher and thus was heated to 600°C and slowly cooled which created a pure alloy of tin and gold. For the $AuSn_2$ and $AuSn_4$ the samples needed to be heated to 500°C and then rapidly cooled and crystalized at 290°C and 240°C, respectively. This process created samples that had the correct crystalline structure (Figure 1).

After the samples had been created, XRD was done to confirm their crystalline structures. The machine used a 5 mm slit and swept two theta angles from 10° to 80°. This was placed against a reference to see where the peaks were located on the spectrum. XPS and UPS were then completed for the samples to see what electronic states they were exhibiting. The use of argon gas was employed to complete a contamination removal and a depth analysis. The UPS measurement enables

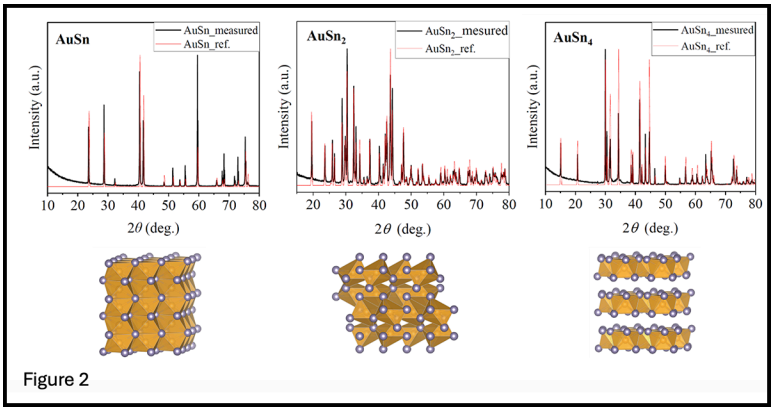


Figure 2

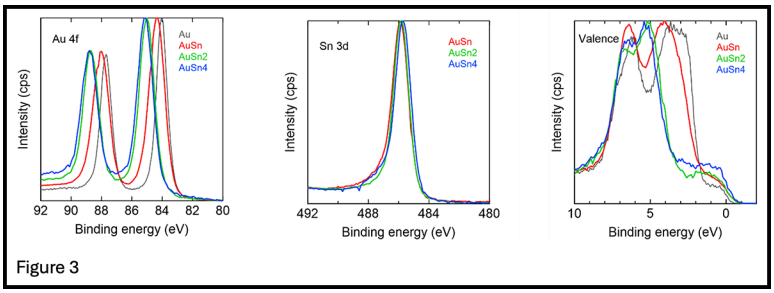
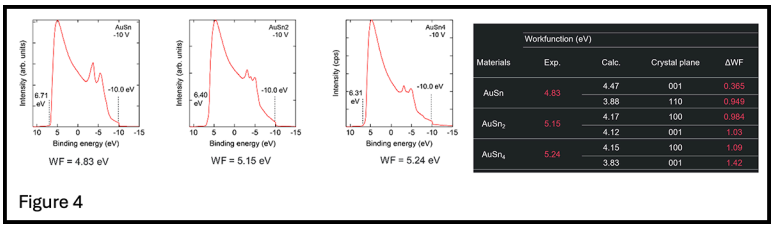


Figure 3



Materials	Workfunction (eV) Exp.	Calc.	Crystal plane	ΔWF
AuSn	4.83	4.47	001	0.365
		3.88	110	0.949
$AuSn_2$	5.15	4.17	100	0.984
		4.12	001	1.03
$AuSn_4$	5.24	4.15	100	1.09
		3.83	001	1.42

Figure 4

position. However, in the valence spectra again it was seen that with an increase of tin the band decreased in width and shifted to higher binding energy (Figure 3).

Additionally, to gain more data on the system, the work function was examined theoretically and experimentally through UPS. It was found that the experimental work functions differed from the theoretical, and the change became more apparent as tin content increased in the sample (Figure 4). This leads to some interesting questions as to why the work function values differ so greatly from the theoretical with the change in tin. Looking more closely at the crystal orientation of each sample it is believed that something is not being explored fully. This leads back to the XPS results and the spectra increasing in binding energy with the increasing tin and the associated hypothesis of the gold and tin acting as cations.

Looking at the materials that have similar physical properties, electrides are front and center. Although with the tin-based intermetallic compounds, the atoms are acting as cations instead of anions. There is still testing and further research to be done to solidify how the material works but it is interesting to note that the tin-based samples are not behaving the same way experimentally as they are theoretically.

to estimate the workfunction values, which is important to create practical electronic devices.

Results and Discussion. From XRD analysis, the reference and experimental data lined up showing that our intermetallic samples are highly pure and crystalline Au-Sn compounds, as designed (Figure 2). After confirming the orientation of the crystal planes, the AuSn sample was examined by XPS which interestingly had a shift towards higher binding energy in the gold spectra compared to the gold reference. This implies that there is an increase of positive charge cations or a decrease in negative charge anions with the addition of tin. Similarly, this also occurred in the valence spectrum where the band was narrower, and the binding energy was shifted higher implying that there is ionic bonding occurring. From both of these observations, it is hypothesized that the gold and tin in AuSn are behaving as cations in the sample.

To further examine the samples and confirm the hypothesis, the $AuSn_2$ and $AuSu_4$ samples were run through XPS and it was found that as the tin content increased in the sample, the binding energy was shifted higher in the gold spectrum. In the tin spectrum the samples seemed to stay consistent in the peak

Conclusions:

In conclusion, this study reveals how the crystal structure and tin content in AuSn, $AuSn_2$ and $AuSn_4$ intermetallic compounds influence their physical properties. Through XRD, XPS and UPS analysis, there were significant shifts in binding energy and work function values observed that deviated from the theoretical predictions. This suggests that there are complex behaviors occurring the material that may be similar to electrides. These finding highlight the need for further research on the compounds to fully understand and optimize the materials for applications in sustainable technologies.

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