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Investigation of the structural and optical properties of ACZTS solid solution

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Presented By:

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Session: Applied Physical Science

Presentation outline

- Introduction
- Experimental details
- Results and discussion
- Conclusion

Introduction

Quaternary Chalcogenide Cu_2ZnSnS_4 material:

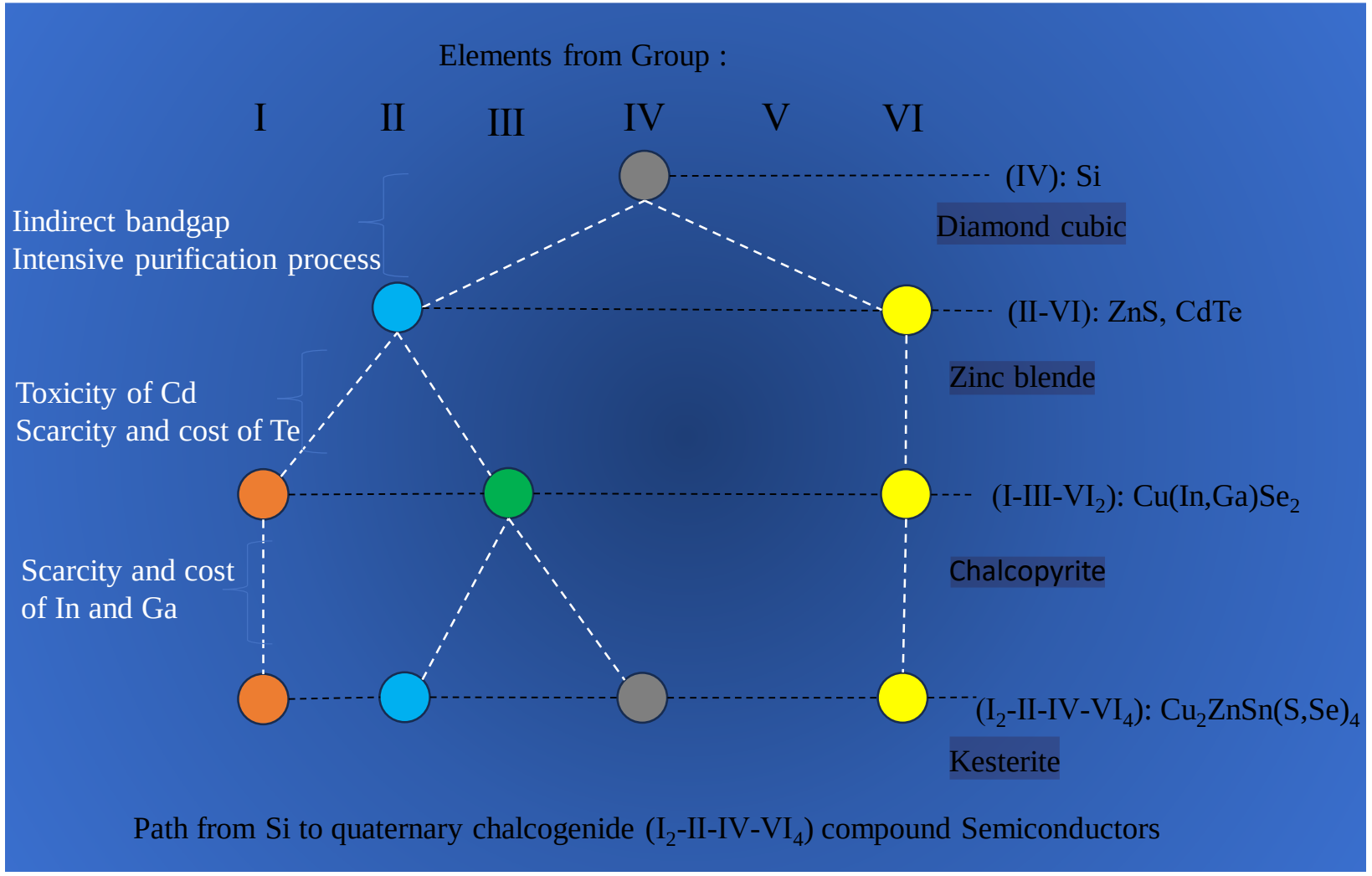
Made from ecofriendly and abundant elements.

Large absorption coefficient ~ 10^4 cm^{-1}.

Direct band gap energy of about 1,5 eV.

Wide tunability of its structural and optical properties through elements substitution.

To focus on the effect of substituting Cu with Ag on the structural and optical properties of the solid solution $(Ag_xCu_{1-x})_2ZnSnS_4$ (ACZTS).

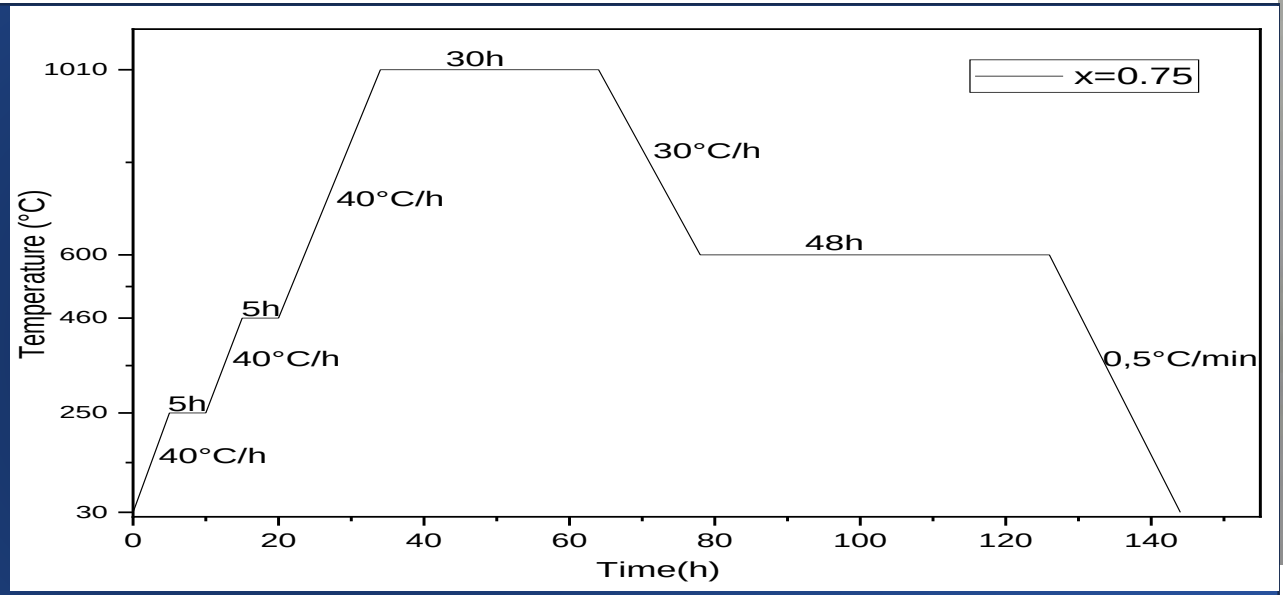


Path from Si to quaternary chalcogenide (I_2-II-IV-VI_4) compound Semiconductors

Experimental details

Polycrystalline $(Ag_xCu_{1-x})_2ZnSnS_4$ x = 0.0 (AC00), 0.25 (AC25), 0.50 (AC50), 0.75 (AC75), 1 (AC100) have been synthesized via solid state reaction as follows :

Sealing a fused quartz ampoule loaded with raw material mixtures under vacuum → Heating the sealed ampoules to above the melting point of the compounds (980-1100°C) → Cooling the ampoule in a controlled manner by lowering the furnace temperature → retrieving the synthesized material (ACZTS)

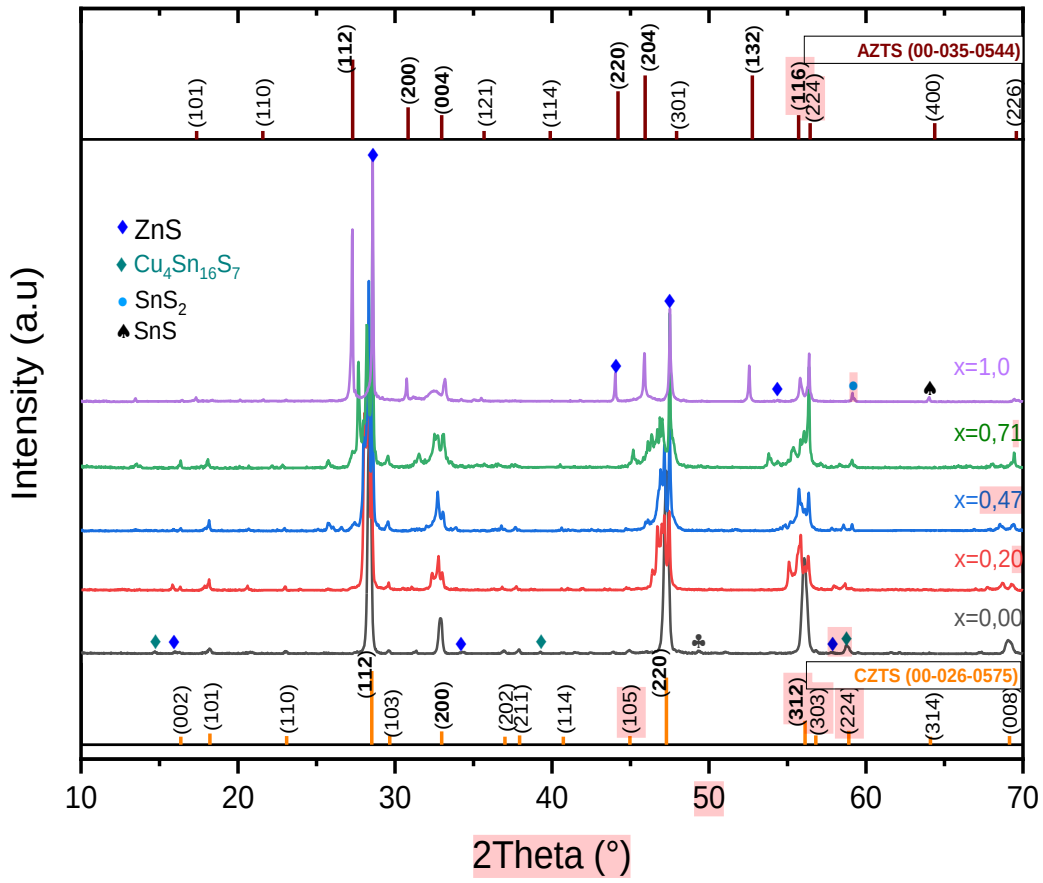


The temperature profile programmed in the electrical tubular furnace

Obtained ingot

Results and discussion

- For x=0 (CZTS), a distinct diffraction lines with the presence of main peaks at (112), (200), (220), (132) and (116) corresponding to the Kesterite CZTS structure.
- The position of diffraction line shifts toward a low angles with the increase of Ag content.
- As x=0.71, the (200), (220) and (312) start splitting up.
- The dominant phase with a kesterite (CZTS) type-structure is gradually shifted into perquitasite-AZTS type structure.
- As x=1 (AZTS), the (004), (204) and (116) peaks associated with tetrahedral perquitasite AZTS type structure appear.
- Secondary phases, mainly (ZnS) in all compositions and others such as CuS, CTS in x=0 and SnS, SnS2 in x=1, are also revealed by XRD analysis.



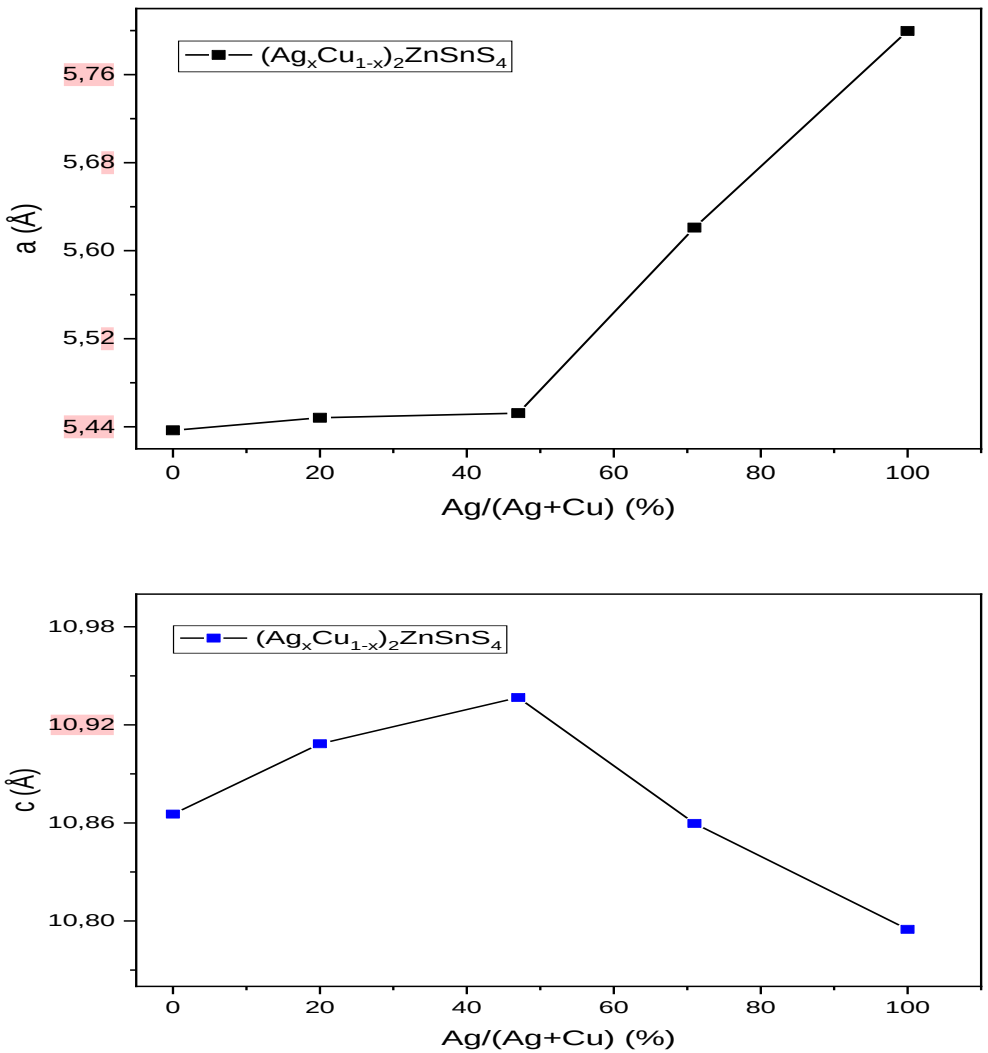
XRD powder analysis of the five synthesized $(Ag_xCu_{1-x})_2ZnSnS_4$ ($0 \leq x \leq 1$) samples

Results and discussion

The lattice parameters (a) and (c) of the obtained (AgxCu1-x)2ZnSnS4 samples as a function of ($0 \leq x \leq 1$) were calculated from the major peaks of XRD patterns ;

$$\frac{1}{d_{hkl}^2} = \frac{h^2 + k^2}{a^2} + \frac{l^2}{c^2}$$

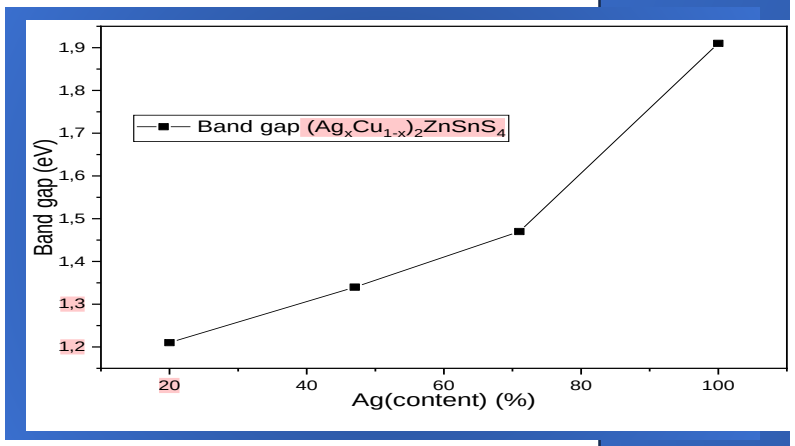
- The lattice constant (a) increases slightly with increasing Ag content from x=0 to x=0.47, and when Ag > 47% the lattice constant (a) undergoes a significant expansion, becoming considerably larger.
- Similarly, the lattice parameter (c) increases slightly as we move from x=0 to x=0.47 compositions, while the latter parameter becomes significantly reduced beyond 47% Ag content.
- The observed trends in lattice constants of $(Ag_xCu_{1-x})_2ZnSnS_4$ deviate from Vegard's law indicating the formation of point defects during synthesis.



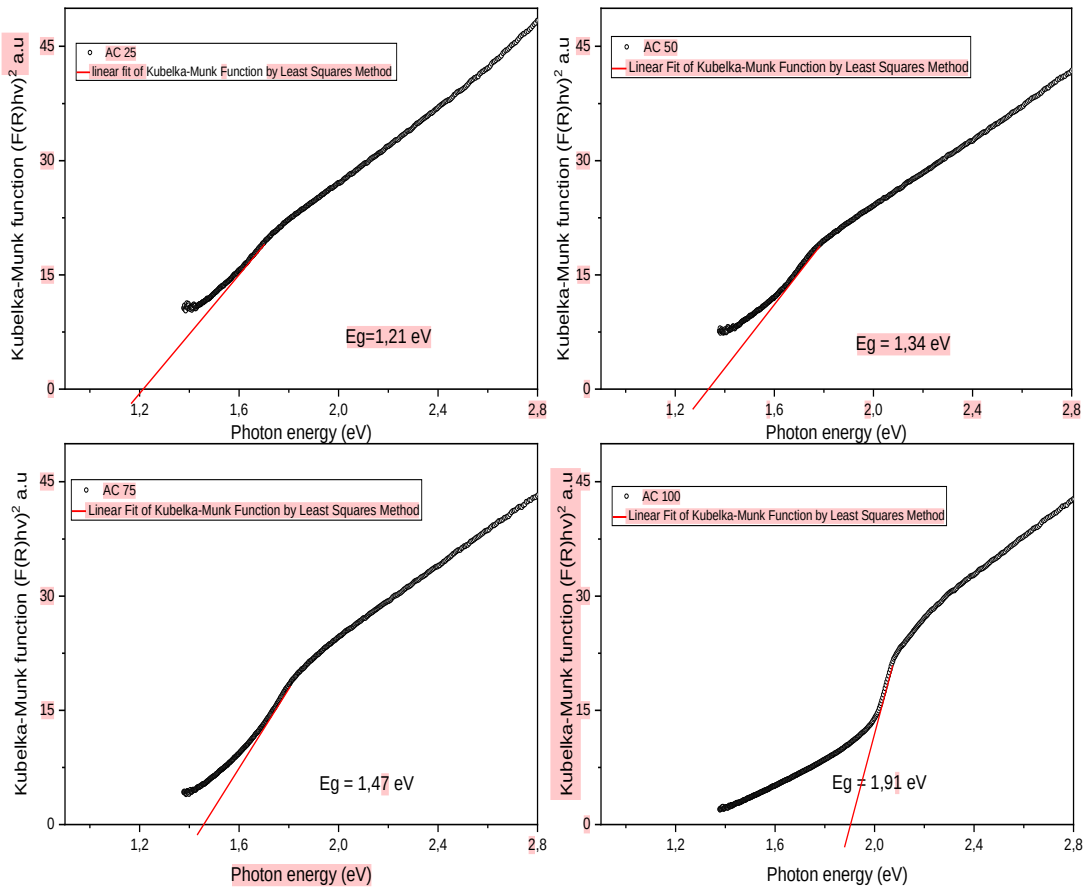
Lattice parameters trend of the obtained (AgxCu1-x)2ZnSnS4 samples

Results and discussion

Optical properties of $(Ag_xCu_{1-x})_2ZnSnS_4$, performed by UV-Vis diffuse reflectance measurements.



- The optical properties could be tuned by varying the Ag content.
- Due to the presence of secondary phases and points defects, the variation of the band gap does not depend linearly on Ag concentrations



Band gaps of $(Ag_xCu_{1-x})_2ZnSnS_4$ from diffuse reflectance spectroscopy measurements

Conclusion

- The objective of this study was to prepare solid solutions of ACZTS by carefully following the steps of the solid state synthesis aiming to investigate the impact of the partial and total substitution of Cu by Ag on the properties of the CZTS absorber properties.

- XRD powder analysis showed a noticeable pattern variation in the structural characteristics of the CZTS lattice. The diffraction lines are slightly shifted to lower angles with increasing Ag content, the perquitasite type AZTS structure peaks appeared in fully substituted compounds, implying that substitution of the Cu site by Ag occurs.

- The lattice constants exhibit non-linear trends that deviate from Vegard's law as a consequence of defects formation during the synthesis, indicating that the formation of a solid solution within the $(Ag_xCu_{1-x})_2ZnSnS_4$ material did not occur as expected.

- UV-Vis diffuse reflectance measurements showed that optical properties could be tuned by varying the Ag content, however, due to the presence of secondary phases, the variation of the band gap does not depend linearly on Ag concentrations.

- Our results provide valuable insights into the effect of Ag substitution on the structural and optical properties of CZTS, and offer directions for further research into the nature of the defects observed in our samples, including additional characterization techniques namely XPS (X-ray photoelectron spectroscopy) and PL (photoluminescence)…

THANK YOU

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