materials proceedings

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Abstract

Structural and Optical Characterization of Mechanochemically Synthesized $CuSbS_2$ †

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† Presented at the Materials 2022, Polytechnic of Leiria, Marinha Grande, Portugal, 10–13 April 2022.

Keywords: chalcostibite; powder technology; mechanochemical synthesis; absorber materials; thin-film solar cells

The present work describes experimental studies related to the characterization of $CuSbS_2$ directly synthesized after 2 h of mechanochemical synthesis (MCS) at 340 rpm, starting from mixtures of elemental powders. X-ray diffraction (XRD) and UV-VIS-NIR spectroscopy were carried out to analyze the crystal structure, degree of crystallinity, crystallite size and optical properties of the mechanochemically synthesized $CuSbS_2$ powders. Rietveld refinement was carried out using Diffrac. TOPAS (Bruker AXS). Thermal stability of the synthesized materials was evaluated by the vacuum thermal heat treatment of the mechanochemically synthesized $CuSbS_2$ powders at 350 °C for 24 h. Furthermore, the $CuSbS_2$ powders were also analyzed by field-emission scanning electron microscopy (FE-SEM), laser diffraction, and differential thermal analysis.

As the Figure 1 shows, all XRD peaks were assigned to the orthorhombic chalcostibite phase with the space group Pnma (COD database file 9003580). This result is significant and demonstrates the direct synthesis of $CuSbS_2$ powders at room temperature after a short-duration MCS process. The absence of any phase transformation with heat treatment at 350 °C/24 h revealed the strong structural stability of the produced phase. The optical bandgap was determined to be around 1.41 eV, in good agreement with the values reported in the literature. This suggests that mechanochemically synthesized $CuSbS_2$ compounds can be considered suitable to be used as absorber materials of thin-film solar cells. Additionally, the obtained results also indicate that the MCS process is a viable and promising route for the preparation of materials for photovoltaic applications.

Citation: Esperto, L.; Figueira, I.; Mascarenhas, J.; Silva, T.P.; Correia, J.B.; Neves, F. Structural and Optical Characterization of Mechanochemically Synthesized $CuSbS_2$. *Mater. Proc.* **2022**, *8*, 65. https://doi.org/10.3390/materproc2022008065

Academic Editors: Geoffrey Mitchell, Nuno Alves, Carla Moura and Joana Coutinho

Published: 13 April 2022

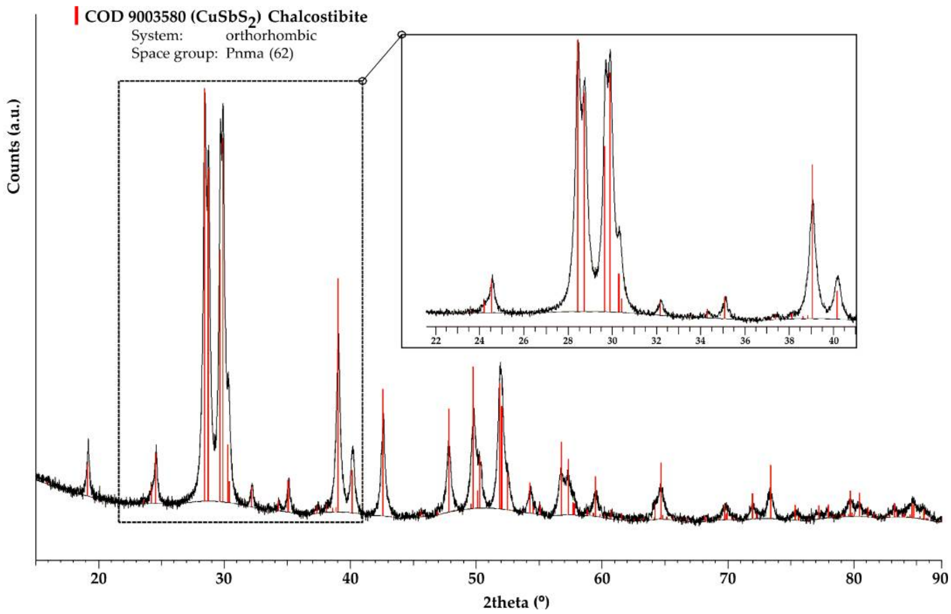

Figure 1. Typical XRD pattern of the $CuSbS_2$ powders produced directly by mechanochemical synthesis.

Author Contributions: Conceptualization, J.B.C. and F.N.; investigation, L.E., I.F., J.M. and T.P.S.; writing—original draft preparation, J.B.C. and F.N.; writing—review and editing, L.E., I.F., J.M., T.P.S., J.B.C. and F.N.; project administration, F.N.; funding acquisition, F.N. All authors have read and agreed to the published version of the manuscript.

Funding: This work is funded by national funds through the FCT–Fundação para a Ciência e a Tecnologia, I.P., under the project PTDC/EAM-PEC/29905/2017 (LocalEnergy project, http://localenergy.lneg.pt, accessed on 2 June 2022).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Acknowledgments: The “Direção Geral de Energia e Geologia” participates as an “External Advisor” in LocalEnergy project.

Conflicts of Interest: The authors declare no conflict of interest.