

CHARACTERIZATION OF TETRAHEDRITE $\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}$ MONOGRAIN MATERIALS GROWN IN MOLTEN CdI_2 AND LiI

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Cd-substituted tetrahedrite $\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}$ (TH-Cd) monograin powders (MGPs) was performed by the molten salt synthesis-growth method using two different fluxes. The influence of nature of the used flux salts on the elemental and phase composition of TH-Cd MGP particles, on their size distribution, morphology, as well as on the rate of particles' agglomeration, was studied. The $\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}$ powder materials were synthesized from CdS (5N) and Cu_2S (5N) and Sb_2S_3 (5N) by isothermal recrystallization method in cadmium iodide (CdI_2) and lithium iodide (LiI) at 495 °C for 336 hours. The mass ratio of precursors to flux salt $m_{\text{TH-Cd}}/m_{\text{flux}}$ was kept 1 : 1. More details about the MGPs growth of TH compound could be found in [1][2].

The X-ray diffraction data of the materials indicated that mainly single phase of tetrahedrite $\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}$ compound was formed in both flux salts. XRD pattern of TH-Cd crystals grown in LiI revealed a shift of all diffraction peaks, lower CdS content and a smaller lattice parameter values in comparison with those formed in CdI_2 ($\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}$ synthesized in LiI : $a=b=c=10.509$ Å and in CdI_2 : $a=b=c=10.512$ Å). Energy dispersive X-ray spectroscopy revealed stoichiometric composition of $\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}$ crystals grown in CdI_2 and Cu-poor grown in LiI . Images of scanning electron microscope showed different morphology of TH-Cd crystals formed in CdI_2 , and LiI . The produced MGPs were used as an absorber material in MGL solar cells with a structure of $\text{ZnO}/\text{CdS}/\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}/\text{graphite}$. The MGL solar cell, based on TH-Cd grown in LiI media showed higher parameters (η of 0.79% was achieved) than the one with TH-Cd grown in CdI_2 (η of 0.13%). Based on these results, we can conclude that Li^+ from the molten flux (LiI) incorporates into the $\text{Cu}_{10}\text{Cd}_2\text{Sb}_4\text{S}_{13}$ crystals structure and most probably partly replacing Cu^+ sites in the lattice forming $\text{Cu}_{10-x}\text{Li}_x\text{Cd}_2\text{Sb}_4\text{S}_{13}$ solid solution.

References

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2. J.Krustok, T. Raadik, R.Kaupmees, F.Ghisani, K.Timmo, M.Altosaar, V.Mikli, and M.Grossberg, 2020, *J. Phys. D. Appl. Phys.*



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