Raman investigations of $Cu_2Mg_xZn_{1-x}SnS_4$ films with different chemical composition

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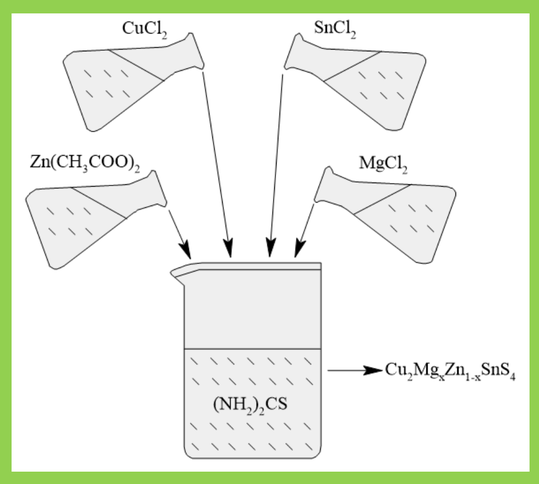
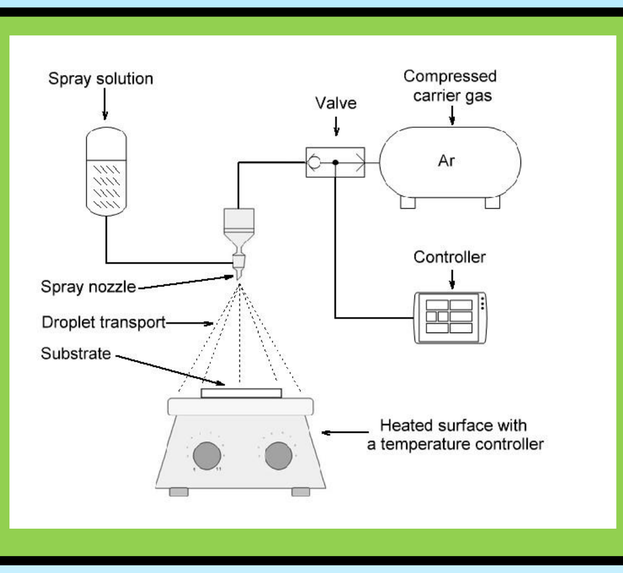
Introduction

Currently, Cu_2ZnSnS_4 is considered a promising material for the absorption layers of solar cells (SC) of the third generation. However, despite a large number of studies, the efficiency of photo converters based on it does not exceed 10%. The main reason for this is the low value of the no-load voltage compared to the width of the bandgap of the material, which is associated with the formation of anti-structural defects Sn_{Zn}. One way to overcome this disorder is to replace Zn with Mg in the crystal lattice of the semiconductor, giving new options based on the $Cu_2Mg_xZn_{1-x}SnS_4$ compounds.

Methods



To create a precursor, saline solutions in stoichiometric amounts of $CuCl_2$: $Zn(CH_3COO)_2$: $MgCl_2$: $SnCl_2$: $(NH_2)_2CS$ = 2 : 1-*x* : *x* : 1 : 4 were slowly added to the thiourea solution. As a result of mixing the initial solutions, transparent molecular precursors with an x value in the range from 0 to 0.4 were obtained. The films were obtained by application using the technique of spray pyrolysis.



Results

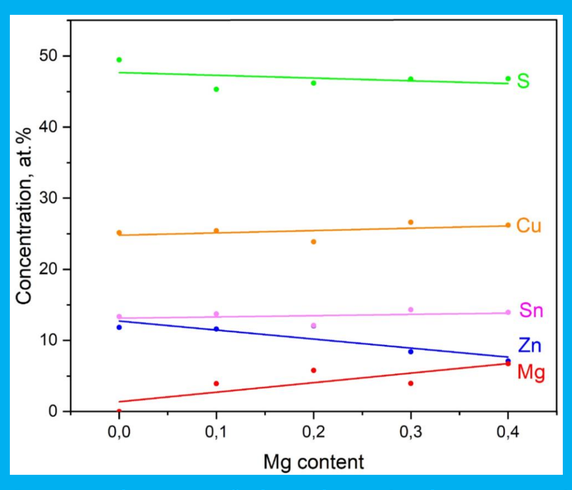


Fig. 1 - Dependence of the chemical composition of $Cu_2Mg_xZn_{1-x}SnS_4$ films

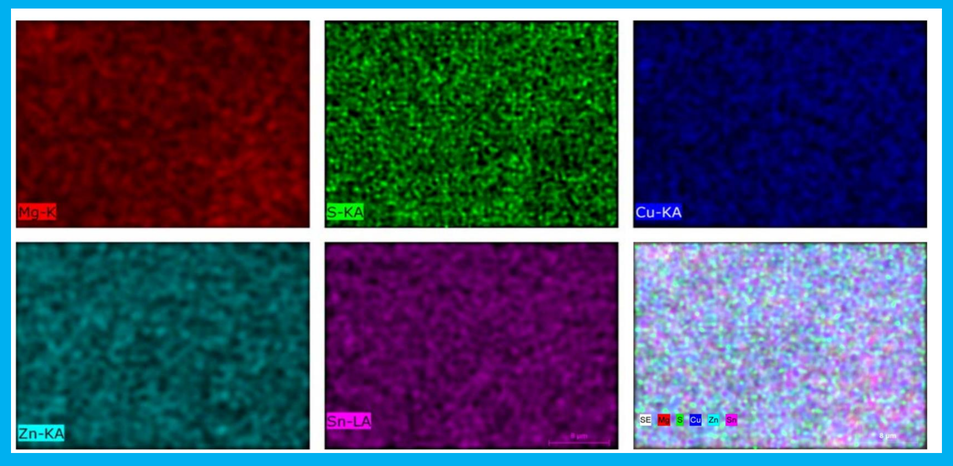


Fig. 2 - Elemental distribution maps of the sample $Cu_2Mg_{0,4}Zn_{0,6}SnS_4$ surfaces

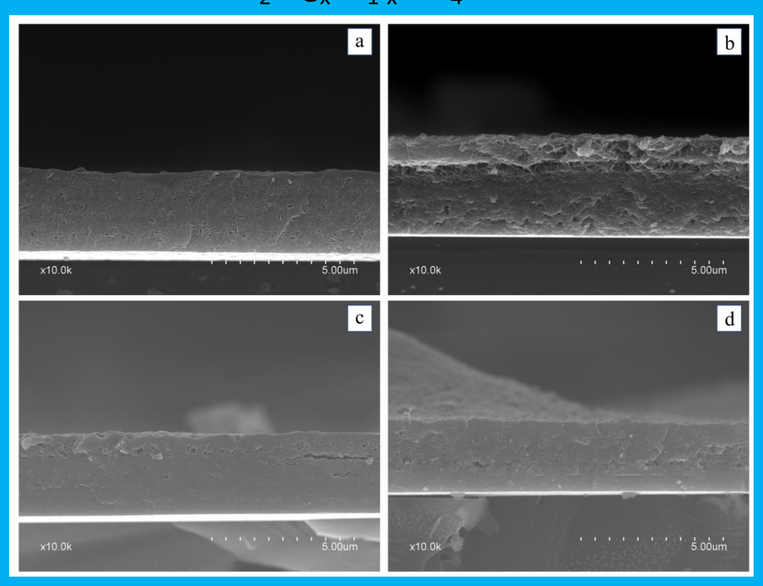


Fig. 3 - Electron microscopy images of the cross-sections of $Cu_2Mg_xZn_{1-x}SnS_4$ films: x = 0.1 (a); x = 0.2 (b); x = 0.3 (c); x = 0.4 (d)

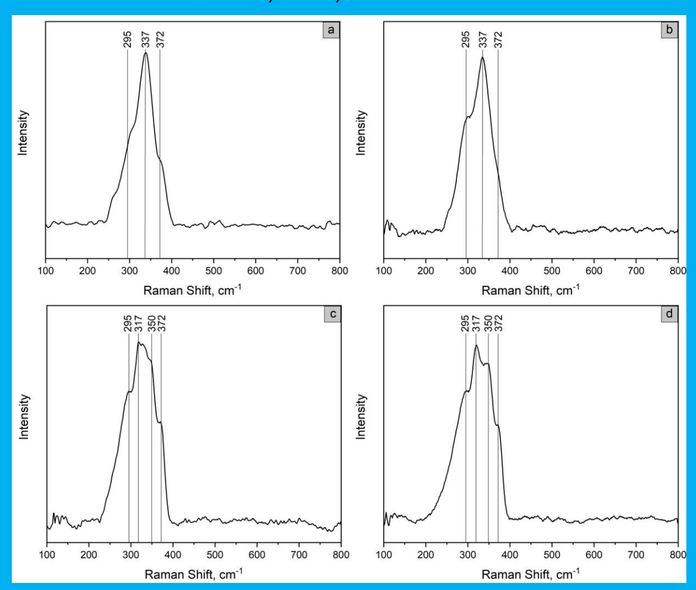


Fig. 4 - Raman spectra of films of solid solutions $Cu_2Mg_xZn_{1-}xSnS_4$ doped with magnesium : x = 0.1 (a); x = 0.2 (b); x = 0.3 (c); x = 0.4 (d)

Conclusion

- Studies of the elemental composition of the films the following values of the concentrations of C_{Mg} atoms in the samples: 0%, 3.91%, 5.77%, 3.94%, 6.70%;
- The Raman investigation of samples with Mg nominal content up to 20% shows that they have three main peaks at frequencies of 295 cm^{-1}, 337 cm^{-1}, and 372 cm^{-1}, which correspond to the reference data for pure kesterite compounds;
- With a further increase in Mg content, a new peak intensity appeared at a frequency of 350 cm^{-1}, which may indicate the presence of a secondary phase of Cu_2SnS_4;
- The shift of the A1 peak from the frequency of 337 cm^{-1} to the frequency of 317 cm^{-1} was detected, this shift is explained by the replacement of smaller radii of Zn^{2+} ions with larger Mg^{2+} ions.