Physico-Chemical nanomaterials science

Optical and structure properties of Cu_2ZnSnS_4 grown by DC magnetron sputtering with extended linear sizes

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Cu_2ZnSnS_4 (CZTS) is a promising light absorber material for the production of thin film solar cells (TF SCs) due to its desirable direct optical gap of 1.5 eV and large band-to-band optical absorption coefficient (~10^5 cm^{-1}). All constituents of CZTS used to utilized in processing are non-toxic and abundant in the earth crust with contrast to well studied CdTe and $Cu_2In(Ga)S(Se)_2$ absorbers. The conversion efficiency record of CZTS-based TF SCs reaches value of 12.6% [1], that it is not enough for industrial production. The aim of this work was to investigate the optical properties of CZTS TF grown by DC sputtering of metallic precursors on linear extended substrates in 40 cm of width and 40 cm of height.

The obtained materials are thoroughly characterized by X-ray diffraction, microscopic and spectroscopic methods. The Raman spectrum shows two dominant peaks at 287 cm^{-1} and 338 cm^{-1}, that are corresponded with A symmetry modes of the kesterite like structure (space group). From the fitting of Raman spectra by a setting of Lorentzian components we can conclude that at the low-frequency side of the most intense band (338 cm^{-1}) a weaker component at about 332 cm^{-1} is observed. Most probably this Raman band is related to disordered Zn and Cu atoms in CZTS lattice, as was discussed in [2]. We assume this disordering is caused by so-called anti-sites defects, such as Zn atoms on the place of Cu (Cu_{Zn}). The occurrence of this defect is possible in samples with depleted content of Cu and Zn excess. The reduction of concentration of Cu in these samples was confirmed by the elemental analysis. Thus the CZTS based TF absorber layer with the kesterite structure were obtained on substrate with extended linear sizes.

1. *Wang W., Winkler M.T., Gunawan O., Gokmen T., Todorov T.K., Zhu Y., Mitzi D.B.* Device characteristics of CZTSSe thin-film solar cells with 12.6% efficiency // Adv. Energy Mater.-2014.-**4**, N 7.- P. 1-5.

2. *Fontane X., Izquierdo-Rosa V., Saucedo E., Schorr S., Yukhymchuk V.O., Valakh M.Ya., Perez-Rodriguez A., Morante J.R.* Vibrational properties of stannite and kesterite type compounds: Raman scattering analysis of $Cu_2(Fe,Zn)SnS_4$ // J. Alloys and Comp.-2012.-**539**.-P. 190-194.