Physico-Chemical nanomaterials science

Optical and crystallographic properties of $Cu_2ZnSnSe_4$ thin films

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The semiconductor $Cu_2ZnSnSe_4$ (CZTSe) is one of the most promising earth-abundant compounds for low-cost solar cells. One of the complex problem on this way deals with cation disorder and non-stoichiometry in this material, which can lead to change of the main phase as well as formation of secondary phases. The cation disorder in CZTSe thin films grown by flash evaporation of ZnSe, CuSe and SnSe binary compounds is studied in this work by Raman spectroscopy and X-ray diffraction. As a measure of cation disorder the intensity, half-width and relative intensity of the Raman band peaked at 184 cm^{-1} is analysed. Comparison of the spectra of samples grown at different conditions shows that the relative intensity of the defect peak at 184 cm^{-1} correlates with the previously reported theoretical prediction about enhancement of antisite defect formation in CZTSe under “Cu-poor, Zn-rich” conditions.

The aim of this work was to determine the type of crystalline structure, composition homogeneity and identification of possible secondary phases in CZTSe films formed on glass substrate covered with a thin layer of molibdenium.

Based on the experimental data and appropriate structural model calculation of the relative intensity of the reflections was calculated and the parameters of the elemental cell refined (Table 1).

Table 1. Lattice parameters and Raman peaks A mode of CZTSe thin films.

	film thickness,nm				Raman peak, cm^{-1}	
	190	5,6894	11,3358	0,9962	194	
	350	5,6771	11,2682	0,9924	191	
	440	5,6728	11,2503	0,9916	189	

Based on frequencies characteristic Raman peaks, related to fully symmetric vibrations of CZTSe [2], the kesterite structure of the samples is established.

1. *Siebentritt S., Schorr S.* Prog. Phot. Res. Appl.- 2012.-**20**.- P. 512.
2. *Sheleg A.U., Hurtavy V.G., Mudryi A.V., et., al.* J. Appl. Spectr.-2014.-**81**, N 5.-P. 776.