Physico-Chemical nanomaterials science

Optically induced structural transformation in Cu_2ZnSnS_4 thin films

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Recently Cu_2ZnSnS_4 (CZTS) and similar quaternary chalcogenides have received considerable attention as potential materials for new-generation thin-film solar cells. The reasons for their appeal are their suitable direct band gap energy of about 1.5 eV, large optical absorption coefficient of 10^4–10^5 cm^{-1}, and the fact that all constituents of CZTS are abundant in the Earth's crust, non-expensive and non-toxic. During last decade the efficiency of CZTSSe-based solar cells has been improved significantly and has reached 12.6% [1].

The aim of this work was to investigate the optically induced structural transformation of CZTS thin films were deposited by flash evaporation of ZnS, CuS and SnS binary compounds in powder form onto molybdenum-coated glass substrates at nominal substrate temperatures, T_{sub}, of 100 or 350°C. The obtained materials are thoroughly characterized by microscopic and spectroscopic methods. One of the complex problem on this way deals with its stoichiometry.

In this work Raman spectra of Cu-rich CZTS thin films are discussed in connection with the non-stoichiometric composition and disordering within the cation sublattice of the kesterite. The shift of the main A-peak in Raman spectra from 338 to 332 cm^{-1} and its broadening are attributed here to transition from the kesterite ($I\bar{4}$-symmetry) to the disordered kesterite structure ($I\bar{4}2m$-symmetry) [2]. It is shown that this transition may also be driven by an intense light, which could stimulate transformation of Cu^+-ion to Cu^{2+}-ions and facilitates generation of Cu_{Zn}-defects on 2d-crystallographic positions.

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. *Valakh M.Ya., Dzhagan V.M., Babichuk I.S., Fontane X., Perez-Rodriquez A., Schorr S.* Optically induced structural transformation in disordered kesterite Cu_2ZnSnS_4 // JETP Letters.-2013.-**98**, N. 5.-P. 255–258.