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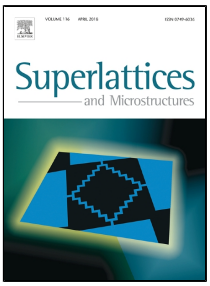

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Sodium doping mechanism on sol-gel processed kesterite Cu_2ZnSnS_4 thin films

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Abstract

Alkali metal doping represents one of the main ways to achieve high-efficiency CIGS solar cells. Since Kesterites are a promising alternative to CIGS based thin films, in this paper, we have investigated the impact of heavy sodium-doping on sol-gel processed CZTS thin films. CZTS solutions were prepared using NaCl as sodium source for doping. Different NaCl to CZTS molar ratios – (0%, 10%, 20% and 30%) were employed. The solutions were then spin coated on clean glass substrates and immediately preheated on a hot plate and subsequently sulfurized in a tubular furnace. Based on the obtained results, 10% molar doping was found to have the best structural quality as proved by XRD and Raman spectroscopy. On the other hand, we also observed that the band gap decreases from 1.45eV down to 1.34eV with increasing sodium-doping from 0% to 30% molar doping, respectively. We used heavily Na-doped CZTS in order to compare our experimental results to theoretical calculations given by density functional theory. This comparison leads to evidence of interstitial sodium doping as dominant model rather than substitution, since the doping expands the volume of the unit cell and reduces the optical band gap, contrary to CIS where the sodium substitution doping is the principal mode.

Keywords: CZTS, Kesterite, Sol-gel, Na-doped.

I. Introduction

Kesterite Cu_2ZnSnS_4 (CZTS) is quaternary semiconductor constituted by non-toxic and Earth abundant materials and it is considered an alternative to the well-known $Cu(In,Ga)Se_2$(CIGS) material. It is made by substitution of In/Ga in CIGS system by Zn/Sn, which make it a potential candidate for terawatt production [1][2]. Despite the similarities between CZTS and CIGS, such as crystal structure, optical band gap (E_g), absorption coefficient and device