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PII: S0040-6090(17)30195-5
DOI: doi: 10.1016/j.tsf.2017.03.020
Reference: TSF 35868

To appear in: *Thin Solid Films*

Received date: 3 June 2016
Revised date: 10 March 2017
Accepted date: 10 March 2017

Please cite this article as: Tsuyoshi Maeda, Chiyuan Zhao, Takahiro Wada , Crystallographic, optical, and electronic properties of (Cu,Li)InS2 system. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Tsf(2017), doi: 10.1016/j.tsf.2017.03.020

Crystallographic, optical, and electronic properties of (Cu,Li)InS_2 system

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Abstract

To investigate the effect of a lithium doping in chalcopyrite-type $CuInS_2$ on its crystallographic and optical properties, we prepared (Cu,Li)InS_2 samples by a mechanochemical process and post-heating at 550^{o}C in H_2S gas. The single-phase chalcopyrite-type $(Cu_{1-x}Li_x)InS_2$ solid solution could be obtained for the samples with $0.0 \leq x \leq 0.10$. The lattice constants *a* and *c* of tetragonal chalcopyrite-type $(Cu_{1-x}Li_x)InS_2$ solid solution increase with increasing Li content. The band gap energy of the $(Cu_{1-x}Li_x)InS_2$ solid solution linearly increased from 1.44 eV of $CuInS_2$ (x = 0.0) to 1.54 eV of $(Cu_{0.90}Li_{0.10})InS_2$ (x = 0.10). We performed first-principles band structure calculations for chalcopyrite-type $(Cu_{1-x}Li_x)InS_2$, using the HSE06 nonlocal screened hybrid density functional. Theoretically, the band-gap energies of the $(Cu_{1-x}Li_x)InS_2$ increase with increasing Li content. The energy levels of the valence band maxima (VBMs) were estimated from the ionization energy measured by photoemission yield spectroscopy. The ionization energy of chalcopyrite-type $(Cu_{1-x}Li_x)InS_2$ solid solutions increased from 5.45 eV of $CuInS_2$ (x = 0.0) to 5.79 eV of $(Cu_{0.90}Li_{0.10})InS_2$ (x = 0.10). The energy level of the VBM of the $(Cu_{1-x}Li_x)InS_2$ solid solution considerably decreases with increasing Li content, x. The conduction band minimum (CBM) level of the $(Cu_{1-x}Li_x)InS_2$ solid solution also decreases with increasing Li content. The Li-doping in $CuInS_2$ is expected to be useful for decreasing the VBM of $CuInS_2$ absorber and increasing the band-gap energy of $CuInS_2$ absorber without increasing the CBM level.

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