Low-cost synthesis of Mn-substituted stannite analogue $Cu_2(Fe_{x-1}Mn_x)SnS_4$ for solar cells

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Semiconductor compounds are amongst the most promising material options for thin film solar cells. The semiconductor based on stannite structure Cu_2FeSnS_4 (CFTS) has recently attracted attention. It is based on Earth-abundant and environmentally friendly constituents and its properties are similar to already commercialized direct gap absorbers such as CdTe and $Cu(In,Ga)Se_2$ (CIGSe). Stannite crystal structure allows for multiple substitutions, including that of Mn for Fe.

The aims of this study are synthesis and characterization of $Cu_2(Fe_{x-1}Mn_x)SnS_4$ (CFMTS) solid solution series with respect to the variation of crystal structure and properties useful to photovoltaic technology. Six members of the series have been synthesized by hydrothermal reactions in an autoclave at 180 ^oC. The structural, morphological, chemical and optical properties of as-synthesized CFMTS nanospheres were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM) with energy dispersive X-ray spectrometry (EDS), micro-Raman spectroscopy, and Fourier-transform infrared spectroscopy (FTIR).

All the product precipitated as the aggregates of nanocrystals displaying characteristic, concentric spherical morphology with average grain size ca. 1.0±0.5 μm. Raman and FTIR spectroscopies confirm the phase purity. The XRD patterns correspond to stannite structure shifted systematically with the extent of Mn substitution. The increase of the lattice parameters and lattice volume is in agreement with the increasing ionic radius of the substituting element (Mn2+ = 83 pm, Fe2+ = 78 pm). The analysis using UV-vis spectroscopy, however, reveals multiple perturbations in inner crystalline structure which remain to be explained. Still, there is potential that partial Mn substitution in a synthetic analogue of stannite may allow for improvement of photoelectric and photocatalytic properties of this alternative photovoltaic material.

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