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ACCEPTED MANUSCRIPT

In-Situ X-ray Diffraction Analysis of the Recrystallization Process in Cu₂ZnSnS₄ Nano Particles Synthesized by Hot-Injection

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Abstract

Kesterite Cu₂ZnSnS₄ (CZTS) is a promising material for thin film solar cell applications. The biggest advantages of this compound lie in the abundancy and non-toxicity of the contained elements. Low temperature hot injection synthesis can provide an economic way to produce CZTS nano particles for application in solution processed solar cells. Powder X-ray diffraction (PXRD) measurements on the assynthesised particles suggest that the crystal structure is cubic and can be best described as sphalerite-like. This means that the cations in the CZTS are statistically distributed on the cation sites of the crystal lattice rather than well-ordered like in the tetragonal kesterite structure. An in-situ PXRD measurement while annealing the particles up to 550° C revealed a recrystallization process that transforms the structure from cubic to tetragonal meaning an ordering of the cations.

1. Introduction

In recent research for thin film photovoltaics, the chalcogenide material Cu₂ZnSnS₄ (CZTS) has <u>attracted interest</u> as a potential future absorber material in photovoltaics.

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