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Chemical crystallographic investigation on Cu_2S-In_2S_3-Ga_2S_3 ternary system

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Abstract

Sulfide chalcopyrites $Cu(In,Ga)S_2$ (CIGS) have been proposed as top cell for tandem solar devices with silicon as bottom cell. In that context, the knowledge of the Cu_2S-In_2S_3-Ga_2S_3 pseudo-ternary system is of prime importance. This study presents an overall investigation of this system on the basis of a chemical crystallographic approach on bulk materials. Particular attention was paid on the copper-poor side of the so-called stoichiometric $CuInS_2$-$CuGaS_2$ line. Based on our investigations, it turns out that the sulfide CIGS system is much more structurally complex than the selenide $Cu(In,Ga)Se_2$ one (CIGSe). Especially, the adaptability of the chalcopyrite structure towards Cu deficiency is significantly lower for the sulfides than for the selenide counterparts. Correlatively, a large 2-phase domain exists between the $CuInS_2$-$CuGaS_2$ line and the very copper-poor region ($Cu(In,Ga)_3S_5$ and $Cu(In,Ga)_5S_8$). Additionally, the crystal structures of these very copper-poor compounds contain [InS_6] octahedra and then are totally different than the chalcopyrite structure. These features could explain why CIGS-based-solar cells are, up to now, less efficient than the CIGSe ones.

1. Introduction

In the last decades, photovoltaic industry has grown rapidly and power conversion efficiency of several technologies approach now the Shockley Queisser (SQ) limit (e.g. over 26 % for silicon solar cell [1]). To overpass the SQ limit, tandem solar cells in which a wide