

On the role of sodium and copper off-stoichiometry in Cu(In,Ga)S₂ for photovoltaic applications: Insights from the Investigation of more than 500 samples

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December 23, 2022

Abstract

The present article discusses the investigation of CuIn_{1-x}Ga_xS₂ (CIGS) thin films for photovoltaic applications. For decades, a Cu-rich composition has been used to create solar cells with efficiencies of up to 13.5%; however, interest in chalcopyrite sulfide has recently been revived due to its high and adjustable bandgap, making it a serious candidate as a top cell in tandem configurations. Although chalcopyrite selenides share many properties with CIGS thin films, crucial differences have been reported. To further understand these materials, we studied more than 500 samples of absorbers and resulting solar cells. First, we found that the compositional window for obtaining single-phase CIGS thin films with a 3-stage co-evaporation process is very narrow. Second, we reported that a combination of low copper content and sodium addition during growth is required to maximize the Photoluminescence intensity (*i.e.* to minimize the absorber-related open-circuit voltage losses). Finally, we showed that solar cell performance and stability depend not only on absorber quality but also on phenomena at interfaces (absorber/buffer and grain boundaries). Altogether, we formulate growth recommendations for the manufacture of stable CIGS/CdS solar cells with state-of-the-art efficiency.

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