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Nucleation and growth of thin chalcopyrite films during reactive magnetron co-sputtering

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Abstract
Ternary chalcopyrite semiconductors Cu(In,Ga)S(e)$_2$ have attracted great interest owing to their exceptional material characteristics and theoretically possible solar conversion efficiencies around 30%. While for the selenides Cu(In,Ga)Se$_2$ solar cell efficiencies of more than 20 % have been demonstrated, so far, the highest efficiency of Cu(In,Ga)S$_2$ (CIGS) solar cells is less than 13%. In order to reach higher efficiencies, the CIGS film properties have to be optimized and a detailed understanding of their nucleation and growth mechanism is needed. In this paper, polycrystalline thin film Cu(In,Ga)S$_2$ absorbers have been deposited by reactive magnetron co-sputtering from copper-gallium alloy and indium targets in argon-hydrogen sulfide mixtures, which offers the advantage of a one-step process. The nucleation and growth stages of Cu(In,Ga)S$_2$ films on Mo, TiN and other back contacts on glass substrates were studied by X-ray diffraction (XRD), atomic force microscopy (AFM as well as C-AFM), and scanning electron microscopy (SEM) equipped with energy dispersive X-ray spectroscopy(EDX). The influence of process parameters such as substrate temperature, total sputtering pressure and the energy of the particles on the structure, morphology, intrinsic electrical and optical properties were investigated. From the AFM data the surface roughness and the grain size distributions were determined for different film thicknesses and deposition recipes. Starting the deposition at room temperature, the mean grain size increases only slightly from 35 nm to 50 nm with increasing deposition time, i.e., film thickness. An abrupt increase in the grain size from 57 nm to 400 nm occurs during the heating up stage of the deposition recipes. Also, the surface roughness increases with the sputtering time. The results of the film nucleation and growth will be related to the electrical properties of thin film solar cells, prepared from these films.

Keywords
CIGS
Reactive magnetron sputtering
Nucleation
Thin film growth
Atomic force microscopy