Materials Proceedings

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Proceedings

Surface X-ray Diffraction Study of a Bi-Layer Junction Based on Cu and Cd Sulfides for Photovoltaic Applications †

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† Presented at the 2nd Coatings and Interfaces Web Conference, 15–31 May 2020; Available online: https://ciwc2020.sciforum.net/.

Published: 14 May 2020

Abstract: The development of new-generation photovoltaic devices through more sustainable production techniques and materials is driven by the need to contain the threats to the biosphere while guaranteeing the safety of the supply, accounting for the limited availability of fossil fuels. This study investigates the crystal structure of thin films of chalcogenides, particularly a junction with a p-type (Cu_2S) and an n-type (CdS) layer deposited one on top of the other on a Ag(111) substrate, starting from an aqueous solution and by means of electrochemical atomic layer deposition (E-ALD) (the system is denoted by $(Cu_2S)_{60}/(CdS)_{60}$/Ag(111)). The experiment highlights the profound epitaxial relationship existing between the films and the bulk, consequent to the homogenization of the metrics of the CdS and the Cu_2S structures to values commensurate to the surface periodicity of the substrate. Cadmium sulfide develops an elementary cell with crystallographic axes parallel to those of the Ag(111) and parameters |a|, |b| and |c| not found in any of the known mineral phases. The comparison with the wurtzite-type structure of greenockite shows a compensation mechanism related to the strain imposed by the film growth on the crystallographic Ag(111) surface. The positions in the reciprocal space of the Cu_2S reflection is compatible with a pseudo-hexagonal pattern rotated by 30° with respect to the Ag, as already noticed in relation to a Cu_2S/Ag(111) E-ALD deposit (Giaccherini et al., 2017). The Cu_2S **c** axis results parallel to the direction [111] of the Ag substrate and its structure is characterized by the strong occurrence of the 3.963 Å periodicity, which corresponds to the interatomic distance S-S in the triangular CuS_3 groups, the basis of all the mineral $Cu_{2-x}S$ group structures. These data suggest a pseudo-hexagonal chalcocite-like structure with a planarization of S layers (Giaccherini et al., 2017) as a result of the strong epitaxial relationship existing with the CdS below. This study confirms E-ALD as an energy efficient method for the growth of semiconducting heterostructures with tailored properties.

Keywords: SXRD; E-ALD; cadmium sulphide; copper sulphide