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ROLE OF CU CONTENT IN THE CRYSTAL STRUCTURE AND PHASE STABILITY OF EPITAXIAL CU(IN,GA)S_2 FILMS ON GAP/SI(001)

Reference: *E. Bertin et al., Mater Sci in Semicon Proc 166 (2023) 107685*

Collaborations : Institut FOTON, Rice University Houston (USA)
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Contacts:
N. Barreau (IMN): nicolas.barreau@univ-nantes.fr
O. Durand (FOTON) : olivier.durand@insa-rennes.fr

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This study examines the growth condition to obtain a single-phase Cu(In,Ga)S2 (CIGS) chalcopyrite film epitaxially grown by coevaporation on a GaP/Si(001) pseudo-substrate. In particular, we report the structural differences between KCN-etched Cu-rich and Cu-poor CIGS films coevaporated on GaP/Si(001) by 1-stage process. The Cu-poor CIGS film consists of at least three phases; the main crystal is found to be chalcopyrite-ordered, coexisting with In-rich CuIn5S8, and CuAu-ordered CuInS2, all sharing epitaxial relationships with each other and the GaP/Si(001) pseudo-substrate. On the other hand, the Cu-rich CIGS film is single-phase chalcopyrite and displays sharper X-ray diffraction peaks and a lower density of microtwin defects. The elimination of the secondary CuAu-ordered phase with Cu excess is demonstrated. In both films, the chalcopyrite crystal exclusively grows with its c-axis aligned with the out-of-plane direction of Si[001]. This study confirms prior findings on the thermodynamics of Cu–In-Ga-S and the stability of secondary phases. This work paves the way to the future development of CIGS/Si tandem solar cells.

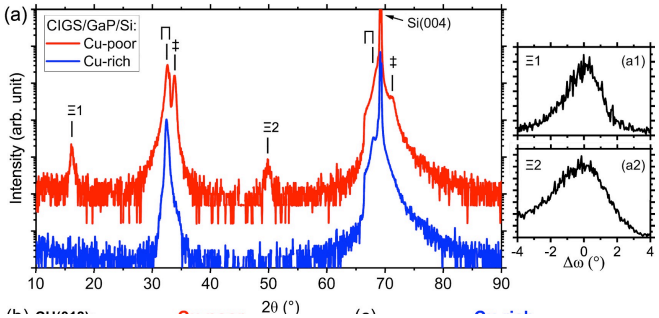
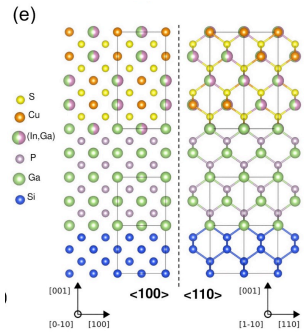


Fig. 2. (a) Low resolution longitudinal ω/2θ scan along the [001] direction of the Si substrate. Transverse ω scans displaying the highly textures nature of the (a1) Ξ1 and (a2) Ξ2 CA peaks. (bc)



Schematics of the crystal stack [41] corresponding to the following epitaxial relationship: CH[100](001)//GaP[100](001)//Si[100](001).