CuGaS₂ thin films prepared from sacrificial epi-GaP layers: toward a new interfacial layer for c-Si/CIGSSe tandems ?

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Cu(In,Ga)(Se,S)₂ chalcopyrites are semiconductors, well adapted to various optoelectronic applications in the visible and NIR thanks to their bandgap ranging from 1.0 eV up to 2.4 eV. Amongst these applications, one can mention photovoltaic conversion. Indeed, single junction cells based on Cu(In,Ga)Se₂ thin films led to outstanding efficiency level and long term stability.

The future generations of PV panels will assuredly imply c-Si/top_cell tandems, where the top_cell could be wide gap halides perovskites, III-V or CIGSSe thin film cells. In this configuration, optimal band gap of the top cell is about 1.6-1.7 eV. Regarding CIGSSe material, such values can be reached by either CuIn_{0.1}Ga_{0.9}Se₂ or CuIn_{0.8}Ga_{0.2}S₂. However, the use of such large bandgap chalcopyrite yields limited device performance. The origins of these limitations are manifolds and include complex phase diagrams, 0D (point defects) and 2D (grain boundaries and hetero-interfaces). Additionally, the hopes for fabricating 2T c-Si/CIGSSe tandems are severely lowered by the poor adhesion of PV-grade CIGSSe layers onto c-Si wafers.

To overcome issues regarding both adhesion and material electro-optical quality, within the frame of the ANR-EPCIS project, we have evaluated the relevance of applying a very thin layer of GaP, epitaxialy grown onto c-Si, before CIGSSe deposition. This interface layer is expected to (*i*) solve adhesion issues of the CIGSSe layer, (*ii*) prevent the diffusion of elements constituting CIGSSe into the c-Si, (*iii*) enhance the epitaxial growth of CIGSSe, thus defect-free layers, since the lattice parameters of GaP and both 1.6 eV CIGSSe compounds are very close.

Our investigations showed that, indeed, the GaP interlayer solves most of those issues when selenide chalcopyrite (CIGSe) is concerned; first tandem devices will be presented in another paper at JNPV (O. Durand *et al., ANR EPCIS project results: CIGS on c-Si Tandem Solar Cell???*). As far as sulfide absorber (*i.e.* Cu(In,Ga)S₂, CIGS) is concerned, the results are drastically different. In this latter case, we have observed that the presence of copper excess during CIGS growth induces partial consumption of the GaP, yielding the formation of CuGaS₂ layer, among others compounds. The chemical reactions resulting in this chaotic interface align with basic thermodynamic considerations. On the one hand side, it suggests impossible to fabricate c-Si/GaP/CIGS tandems. On the other hand, this observation led us to try to fully transform the GaP layer by exclusively supplying copper, under sulfur atmosphere [1]. This approach allowed forming adhesive, well-crystallized thin CuGaS₂ layers onto c-Si, through complete consumption of the GaP layer. Further experiments were then performed with other III-V layers, yielding similar results. The resulting high quality CuGaS₂ can be exploited in diverse optoelectronic domains. Regarding photovoltaics, thanks to its low electron affinity, it can act as electron reflector at the c-Si//CIGSSe interface for efficient tandem devices.

The present contribution aims at explaining the mechanisms behind the III-V consumption, presenting the characteristics of the resulting $CuGaS_2$ layer, and showing our most recent results in that field.

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