

# Epitaxial growth of Cu(In,Ga)S<sub>2</sub> layers on GaP/Si(001) pseudo-substrate and optimization of polycrystalline Cu(In,Ga)S<sub>2</sub> absorbers for tandem Cu(In,Ga)S<sub>2</sub>/Si solar cells

Eugène Bertin<sup>a,b</sup>, Charles Cornet<sup>a</sup>, Maud Jullien<sup>a</sup>, Antoine Létoublon<sup>a</sup>, Polyxeni Tsoulka<sup>b</sup>, Alexandre Crossay<sup>c</sup>, Éric Gautron<sup>b</sup>, Daniel Lincot<sup>c</sup>, Olivier Durand<sup>a</sup>, Nicolas Barreau<sup>b</sup>

<sup>a</sup> Univ Rennes, INSA Rennes, CNRS, Institut FOTON - UMR 6082, F-35000 Rennes, France

<sup>b</sup> Univ Nantes, CNRS, Institut des Matériaux Jean Rouxel – UMR6502, F-44000 Nantes, France.

<sup>c</sup> CNRS, Institut Photovoltaïque d'Île de France, Ecole polytechnique-Institut polytechnique de Paris, Chimie Paristech-PSL, UMR 9006, 18 Boulevard Thomas Gobert, 91120 Palaiseau France

In the family of Cu(In,Ga)(S,Se)<sub>2</sub> compounds, pure-sulfide Cu(In,Ga)S<sub>2</sub> (CIGSu) attracts much attention as its bandgap may be tuned from 1.54 (for CuInS<sub>2</sub>) to 2.43 eV (for CuGaS<sub>2</sub>) [1], making it suitable both for single-junction as well tandem solar cells. Namely, partnered with a crystalline Si (c-Si) bottom cell in a tandem context, CuIn<sub>0.75</sub>Ga<sub>0.25</sub>S<sub>2</sub> displays a near ideal bandgap of 1.7eV for a top cell absorber, while sharing crucial similarities with in GaP in terms of crystal structure and lattice parameters (as shown on Fig. 1).

However, CIGSu solar cells still suffer from low output voltage as compared to their selenide counterparts. This is partly explained by the more complex chemistry of CIGSu [2] as well as higher recombination activity [3] in the bulk, and at buffer/absorber and absorber/Mo interfaces. One improvement pathway to increase minority carrier lifetime consists in eliminating extended crystalline defect, like grain boundaries, where chemical fluctuations may introduce recombination centers [4].

Therein, we work on the epitaxial integration of CIGSu on GaP/Si substrate, which allows simultaneously enhancing the crystalline quality of the CIGSu bulk, and paving the way for monolithic integration of CIGSu top cell onto c-Si bottom cell, in a two terminal configuration. Furthermore, in such a stack, the incorporation of the III-V GaP layer acts as a selective contact for holes.

In parallel, experimental work on standard CuIn<sub>0.75</sub>Ga<sub>0.25</sub>S<sub>2</sub>/Mo/Glass solar cells aims at understanding the combined influence of effective carrier density and thickness of the absorber on the photovoltaic performance of poly-crystalline CIGSu cells, with the help of SCAPS-1D simulations. Moreover, investigations on the replacement of CdS by Zn(O,S) as a junction partner for wide bandgap CIGSu is investigated.

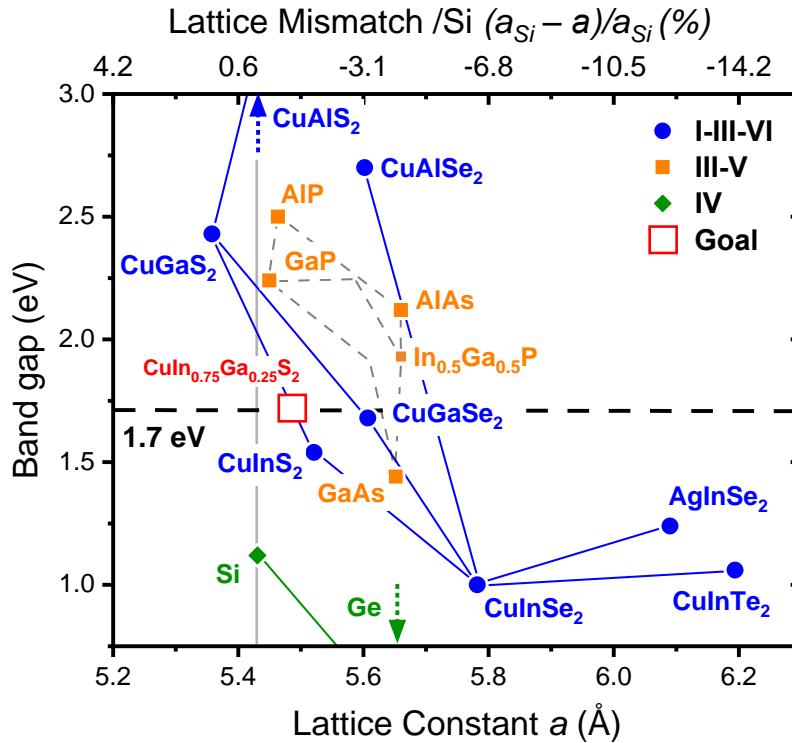


Figure 1: Band gap vs lattice mismatch for chalcopyrite, group IV and III-V semiconductors, whose crystal structure share important similarities. Gallium phosphide GaP is quasi lattice matched with Si. Alloys with the approximate composition  $\text{CuIn}_{0.75}\text{Ga}_{0.25}\text{S}_2$  have near ideal band gap for top cell applications and suitable lattice parameter for epitaxial growth on Si and GaP. Lattice mismatch relative to the lattice constant of Si, is represented on the top x-axis scale.

#### References :

- [1] M. Bär, W. Bohne, J. Röhrich, E. Strub, S. Lindner, M.C. Lux-Steiner, C.-H. Fischer, T.P. Niesen, F. Karg, Determination of the band gap depth profile of the pentenary  $\text{Cu}(\text{In}(1-X)\text{GaX})(\text{SYSe}(1-Y))_2$  chalcopyrite from its composition gradient, *Journal of Applied Physics*. 96 (2004) 3857–3860. <https://doi.org/10.1063/1.1786340>.
- [2] A. Thomere, C. Guillot-Deudon, M. Caldes, R. Bodeux, N. Barreau, S. Jobic, A. Lafond, Chemical crystallographic investigation on  $\text{Cu}_2\text{S-In}_2\text{S}_3\text{-Ga}_2\text{S}_3$  ternary system, *Thin Solid Films*. 665 (2018) 46–50. <https://doi.org/10.1016/j.tsf.2018.09.003>.
- [3] D. Adeleye, A. Lomuscio, M. Sood, S. Siebentritt, Lifetime, quasi-Fermi level splitting and doping concentration of Cu-rich  $\text{CuInS}_2$  absorbers, *Mater. Res. Express*. 8 (2021) 025905. <https://doi.org/10.1088/2053-1591/abe3c1>.
- [4] T. Schwarz, A. Lomuscio, S. Siebentritt, B. Gault, On the chemistry of grain boundaries in  $\text{CuInS}_2$  films, *Nano Energy*. 76 (2020) 105081. <https://doi.org/10.1016/j.nanoen.2020.105081>.

This research was supported by the French National Research Agency EPCIS Project (Grant No. ANR-20-CE05-0038)