

Epitaxial growth of Cu(In,Ga)S₂ thin films on GaP/Si(001) pseudo-substrate: towards Cu(In,Ga)S₂/Si tandem solar cells

Eugène Bertin^{a,b}, Charles Cornet^a, Leo Choubrac^b, Maud Jullien^a, Antoine Létoublon^a, Polyxeni Tsoulka^b, Alexandre Crossay^c, Éric Gautron^b, Sylvie Harel^b, Ludovic Arzel^b, Daniel Lincot^c, Olivier Durand^a, Nicolas Barreau^b

^a Univ Rennes, INSA Rennes, CNRS, Institut FOTON - UMR 6082, F-35000 Rennes, France

^b Nantes Université, CNRS, Institut des Matériaux Jean Rouxel – UMR6502, F-44000 Nantes, France.

^c 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)₂ compounds, pure-sulfide Cu(In,Ga)S₂ (CIGSu) attracts much attention as its bandgap may be tuned from 1.54 (for CuInS₂) to 2.43 eV (for CuGaS₂) [1], making it suitable both for single-junction as well as tandem solar cells. Namely, partnered with a crystalline Si (c-Si) bottom cell in a tandem context, CuIn_{0.75}Ga_{0.25}S₂ displays a near ideal bandgap of 1.7eV for a top cell absorber. In addition, it shares crucial similarities with GaP and Si in terms of crystal structure and lattice parameters (as shown in Fig. 1).

However, CIGSu solar cells still suffer from low output voltage as compared to their selenide counterparts. This deficit is partly explained by the more complex chemistry of CIGSu [2] as well as higher bulk and interface recombination activity [3]. 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].

The epitaxial integration of CIGSu on GaP/Si substrate allows enhancing the crystalline quality of the CIGSu bulk; additionally, it paves the way for adherent monolithic integration CIGSu top cells onto c-Si bottom cells, in a two terminal configuration. In parallel, experimental work on CIGSu/GaP/Si mono-junction solar cells aims at understanding the performances of GaP as a back contact for CIGSu, as well as a potential interconnecting layer.

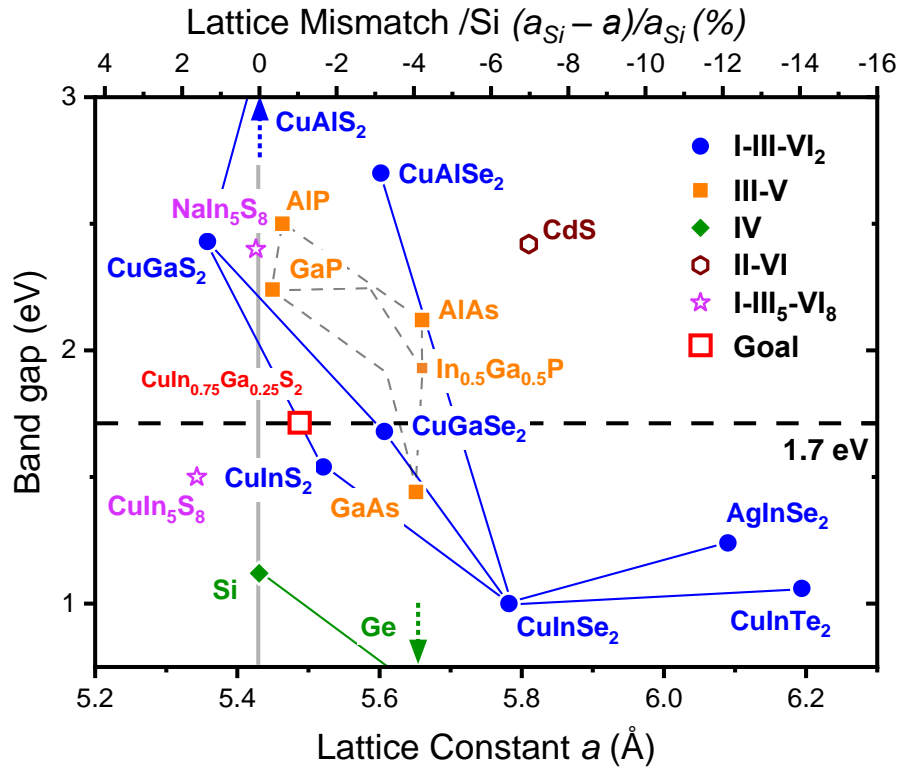


Figure 1: Band gap vs lattice mismatch for chalcopyrite I-III-VI₂, group IV, II-VI and III-V semiconductors, whose crystal structures share important similarities. Gallium phosphide GaP is quasi lattice matched with Si. Alloys with the approximate composition CuIn_{0.75}Ga_{0.25}S₂ have near ideal band gap for top cell applications and suitable lattice parameter for epitaxial growth on Si and GaP. Lattice mismatch relative to 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 Cu(In(1-X)GaX)(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 Cu₂S-In₂S₃-Ga₂S₃ 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 CuInS₂ 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 CuInS₂ 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)