Back to basics:
study of defects in single crystal $CuInS_2$ solar cell absorber material

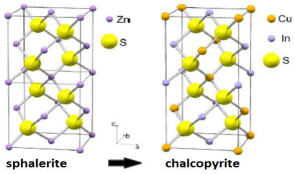
Lisanne Van Puyvelde, P. Matthys, P. Smet, J. Lauwaert, H. Vrielinck
Ghent University, Department of Solid State Sciences, Krijgslaan 281-S1, 9000 Gent, Belgium

Introduction

To improve the efficiency of a solar cell, a good understanding of the defect chemistry of the absorber material is needed. For the fabrication of high efficiency solar cells the ternary chalcopyrite semiconductor $CuInS_2$ is considered to be a promising material. This is due to its optimum band gap of 1.5 eV, its direct type transition structure and its large absorption coefficient above the band gap energy. Up to now, efficiencies of around 12.5 % have been achieved [1] for these types of solar cells.

Structure

$CuInS_2$ belongs to the I-III-VI_2 family of compounds (chalcopyrites) and is derived from the sphalerite lattice by doubling the unit cell to II_2-VI_2. The two group-II atoms are replaced by one group-I atom and one group-III atom.

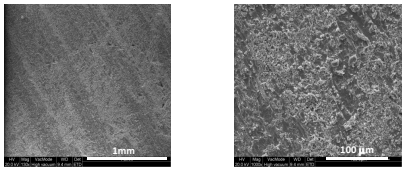


Growth

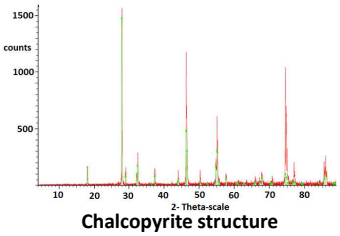
Bridgman growth method: vacuum sealed ampoule with stoichiometric amounts of Cu, In, S is lowered at 1mm/h in a 2 zone oven.
The temperature gradient is 4°C/cm. The upper oven temperature is 1150°C.
To avoid adhesion with the quartz ampoule, a carbon crucible is needed.
The material is p-type for Cu or S rich and n-type for In rich or S poor compositions.

Result: Characterization

SEM:

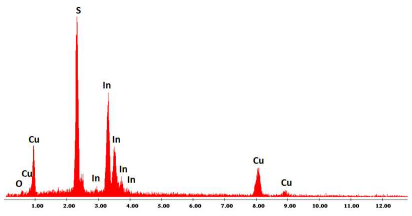


XRD:



Chalcopyrite structure

EDX:



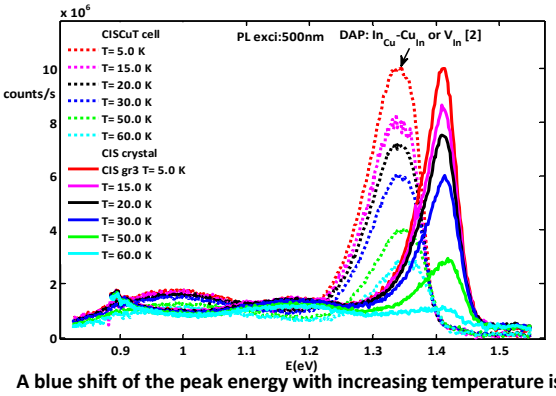
S: 48.46 At%
In: 25.94 At%
Cu: 25.59 At%

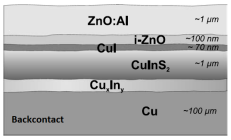
Loss of S is probably due to evaporation during vacuum sealing of the ampoule

Result: Crystal

Result: Photoluminescence spectra

Comparison $CuInS_2$ crystal and $CuInS_2$ on Cu-tape thin film solar cell





A blue shift of the peak energy with increasing temperature is observed for the peaks at highest energy. For the thin film this peak is assigned to the donor-acceptor pair (DAP) recombination, involving In_{Cu}–Cu_{In} antisite or V_{in} defects. The origin of the broad peak at lower energy is unclear.

Conclusion

To study $CuInS_2$ solar cell absorber, crystals can be made by the vertical Bridgman method. Hence, the defect structure of the material can be studied without the influence of the different interfaces in the solar cell.

[1] J. Klaer, Semicond. Sci. Technol. 13 (1998) 1456–1458
[2] J. Van Gheluwe, Thin Solid Films 511 – 512 (2006) 304 – 308