Identification of radiative and non-radiative channels in Cu-poor Cu₂ZnSn(S,Se)₄ solar cells





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Objectives

- Evaluation of the electronic energy levels structure of Cu₂ZnSn(S,Se)₄, with emphasis on the Cu-poor films that optimizes the performance of devices.
- Comparison of two models commonly used in the literature for the discussion of the radiative transitions in kesterites and chalcopyrites.
- Discussion of the role of defects in the limiting factors of the solar cell performance, namely, the V_{oc} parameter, through the identification of the dominant radiative recombination channels.

Methods and techniques

- Photoluminescence in the infrared performed in a 5-300 K temperature range, and excited with visible wavelengths covering more than four orders of magnitude of excitation power
- Electrical conductivity measurements in a Van der Pauw configuration for a 10-350 K temperature range.



Excitation power dependence of a) peak position and b) integrated intensity of the band observed on a Cu-poor Cu_2ZnSnS_4 thin film.



• Hall effect measurements in a Van der Pauw scheme for a 300-350 K temperature range.

Results

- A detailed optical and electrical investigation of CZT(S,Se) thin films have been performed and a high doping level and a strong compensation was identified [1-4].
- The radiative recombination channels are strongly influenced by electrostatic fluctuating potentials which cause the appearance of tails states in the bandgap and fluctuations of the edges of conduction and valence bands along the film (see Fig. 3) [2,3].
- For such semiconductors, bound states for electrons occur just in conduction band tails, created by large enough clusters of donors, and not by single donors [5,6].
- The donor-acceptor pair model cannot be considered for the evaluation of ionization energies in this type of semiconductors [6].
- A deep acceptor level (~280 meV) was identified which contributes significantly for the reduction of the V_{oc} of the final devices [5,7].

Temperature dependence of the a) peak position and b) integrated intensity of the band of a Cu-poor $Cu_2ZnSn(S,Se)_4$ thin film. The inset in b) shows the photoluminescence spectrum measured at 5 K.



Publications

[1] J. P. Leitão et al., *Thin Solid Films*, vol. 519, p. 7390 (2011)
[2] J. P. Leitão et al., *Phys. Rev. B*, vol. 84, p. 024120 (2011)
[3] J. C. González et al., *J. Phys. D: Appl. Phys.*, vol. 46, p. 155107 (2013)
[4] P. M. P. Salomé et al., *J. Mat. Sci.*, vol. 49, p. 7425 (2014)
[5] J. P. Teixeira et al., *Phys. Rev. B*, submitted
[6] J. P. Teixeira et al., *Appl. Phys. Lett.*, submitted
[7] M. G. Sousa et al., *Sol. Energy Mater. Sol. Cells*, vol. 126, p. 101 (2014)

Density of states and energy band diagram for a strongly compensated heavily doped semiconductor.

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