UNIVERSITAT POLITÈCNICA DE CATALUNYA
BARCELONATECH
Escola de Doctorat

Doctoral thesis summary

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Title of the thesis	New processing approaches for Cu2ZnSnSe4-based solar cells
Structural unit	710 - Departament d'Enginyeria Electrònica
Programme	Ingeniería Electrónica
UNESCO codes	221125 | 221190 | 332200 | 330709

(Minimum 1 and maximum 4; see the codes at https://doctorat.upc.edu/academic-management/formsfolder/thesis-registration-and-deposit/unesco-codes)

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The present thesis focuses on the promising semiconductor material kesterite, Cu2ZnSn(S,Se)4, known as CZTS(e), which is used in the second generation of solar cells, generally known as thin film photovoltaics (PV). This material relies on earth-abundant, low-cost and low toxic elements which certainly attract the interest of both research community and industry. Kesterite could replace its well known and already commercialised thin film counterpart, CuIn(1-x)Gax(SySe1-y)2 (CIGS), since it has similar structural and optoelectronic properties and also cell architecture, but does not rely on scarce elements such as In and Ga. In order to achieve a commercial stage kesterite research needs to increase its still limited efficiency (12.6%), which is currently below the 15-18% required value. To achieve this goal, new tailored and customized processing solutions, dealing with major problems of this technology should be investigated and implemented. Moreover, increasing the potential market penetration of kesterite by diversifying its possible applications range can also be an appealing and interesting driver for the industry.

This work focuses on the pure Selenium kesterite, CZTSe, using a versatile and simple sequential two step process to synthesize this absorber. Sputtering and reactive thermal annealing are the techniques chosen to produce CZTSe based solar cells. In addition, two different substrates were used, soda lime glass (SLG) and flexible and light-weight stainless steel (SS) foils. The thesis scope is divided into two interrelated parts:

The first one deals with the proposal of novel and customized approaches to improve CZTSe-based devices performance, mainly using glass substrates. Three innovative processing solutions are developed, proven and included in this work. Two of them deal with the critic Mo back contact region and the third one focuses on the absorber surface. As a result, two original ways to control the decomposition of the back contact interface and the excessive generation of MoSe2 (overselenization) during the thermal treatment along with a chemical passivation route for the CZTSe surface are reported. Intermediate and thin i-ZnO layers and Mo multilayer configurations combined with nanometric MoO2 layers are introduced at the back interface. Likewise, KMnO4/H2SO4 + Na2S aqueous solutions capable of removing ZnSe while passivating the absorber surface are successfully implemented.

The second part of this thesis focuses on the use of flexible and light-weight substrates alternative to conventional and rigid glass based ones. The use of these substrates add an extra value to the already mentioned advantages that kesterite accounts for. A biggest application niche, such as building integration photovoltaics (BIPV), portable consumer electronics, car chassis integration, space applications... etc., along with high throughput roll-to-roll (R2R) industrial manufacturing compatibility, could definitively ease kesterite commercialization.

SS foils have been used successfully in this work, producing the first CZTSe flexible device ever reported in the literature. This thesis includes a detailed optimization of Cr impurity diffusion barriers and Mo back contacts in order to minimize the detrimental effects of metallic substrate impurities in the devices performance.

Additionally, a comparison of different extrinsic alkali doping methods to effectively introduce Na and/or K in flexible and light-weight CZTSe solar cells is also reported. Na doped Mo targets (MoNa), SLG pieces introduced during the annealing, NaF and KF pre-absorber synthesis evaporation (PAS) and post deposition evaporation (PDT) were investigated. We report for the first time a detailed optimization for the use of MoNa layers combined with CZTS(e) technology. In regard to the K investigation, the work developed in this thesis can also be considered as pioneer in the field.

Place	Barcelona	Date	04-02-2016

Signature