Area 2: Thin-film compound semiconductor PV

A COMPARATIVE STUDY OF LIGANDS IN $Cu_2ZnSn(S,Se)_4$ SOLAR CELLS PREPARED FROM NANOPARTICLE INKS

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Cu_2ZnSnS_4 (CZTS) nanoparticle inks annealed in the presence of Se is an attractive thin film solar absorber fabrication technique and has resulted in device efficiencies as high as 9.3% [1]. However, one of the current limitations of this method is the presence of a fine-grain (FG) layer between the $Cu_2ZnSn(S,Se)_4$ (CZTSSe) large grain layer and the back contact. The presence of this FG layer is likely to reduce device performance via carrier recombination through traps, interface states and increased grain boundary density. In our approach, oleylamine (OLA) is used as the capping ligand to prevent the agglomeration of nanoparticles during fabrication (CZTS nanoparticles referred to as CZTS OLA) [2]. The resulting nanoparticle inks are then spin coated on Mo-glass substrates followed by selenization [3,4]. As shown in Figure 1 (a), a bilayer structure is obtained after selenization with a top layer consisting of densely packed large grains (LG) and a bottom layer composed of fine grains. OLA contains long hydrocarbon chains that subsequently carbonize during the selenization process leaving carbon residues in the film and produce the FG layer. It can be seen in Figure 1 (b), high carbon content is found in the FG layer, especially at the interface with the back contact. Alternatively, formamide (FA) is chosen as the solvent in the synthesis of CZTS nanoparticles (referred to as CZTS FA). At high temperature, FA decomposes to form gaseous products to escape from the thin film. Consequently, residual FA in the nanoparticle thin film is less likely to leave carbon residues during the selenization process. As shown in Figure 1 (c, d), the absorber is composed of a single LG CZTSSe layer where the carbon-rich FG layer is eliminated. Although the FG layer is removed, fairly large pores and voids are present at the grain boundaries of CZTS FA films after selenization. As a result, a poor *p*-*n* junction is formed and shunt diode is observed for the device. When a CZTS OLA film is applied on the CZTS FA film, a FG layer is sandwiched between two LG layers as shown in Figure 1 (e). The absorber is densely packed and the dual layer device gives efficiencies up to 4.0% (Figure 1 (f)) which is comparable with single CZTS OLA films. A complete comparative study of the materials properties and solar devices performance is presented.

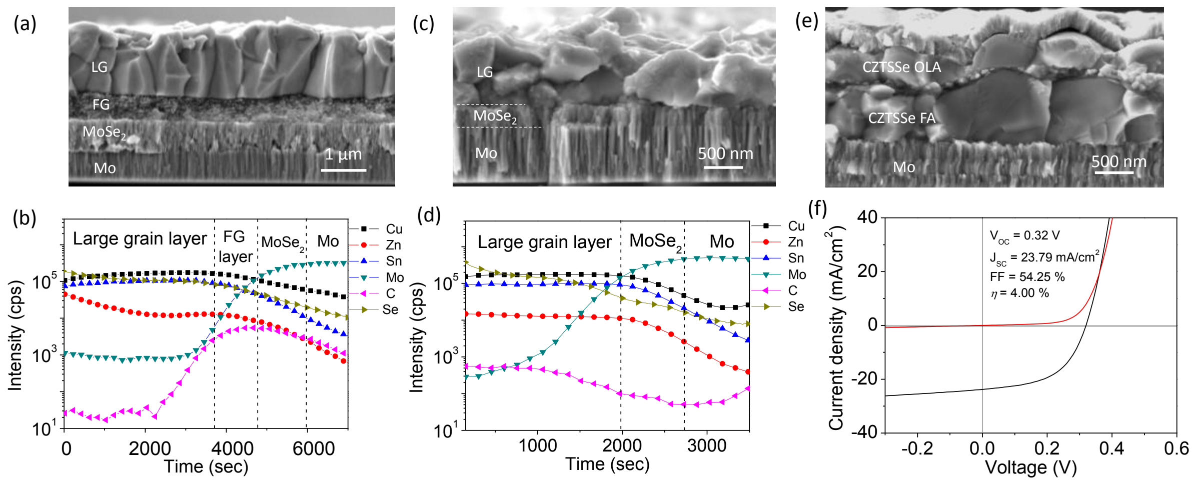

Fig. 1 Cross-sectional SEM images and SIMS depth profiles of selenized absorber made from (a-b) CZTS OLA and (c-d) CZTS FA nanoparticle films. (e) Cross-sectional SEM image of a dual layer device fabricated combining CZTSSe OLA and CZTSSe FA thin film after selenization. (f) *J-V* curve of the dual layer device.

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