Electronic supplementary information

Effects of S and Se contents on the physical and photovoltaic properties of $Cu_2ZnSn(S_X, Se_{1-X})_4$ thin films: 9.45% †

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KEYWORDS

CZTS, CZTSe, CZTSSe, sulfo-selenization, thin film solar cell, kesterites, photovoltaic devices

Supplementary material – 1: Experimental details for the deposition of the CdS buffer layer

Though there are many deposition techniques used to prepare the CdS thin films, chemical bath deposition (CBD) is the simple, inexpensive and reproducible method giving adherent and uniform films. CdS layer was deposited by CBD from a bath containing cadmium sulfate ($CdSO_4$), ammonium hydroxide (NH_4OH), thiourea (NH_2CSNH_2), and DI H_2O. The bath solution used in the in-house CDB CdS process was composed of 732 ml of DI H_2O, 80 ml of NH_4OH ammonium hydroxide, 100 ml of cadmium sulfate (0.015 M $CdSO_4$), and 50 ml of thiourea (1.5 M NH_2CSNH_2). The pH range is commonly 11-11.5 in thin process. A water-heated vessel was used to contain the bath solution, which was constantly stirred by a digital overhead stirrer during the deposition process. The solution is heated by bath with continuous stirring to the required temperature of deposition, and the temperature is controlled to within ± 1 °C at 80 °C. After growing for 7 min, the film was ultrasonically cleaned in deionized water to remove any loosely adhered particles.

Supplementary material – 2: Scanning electron microscopy (SEM) images of the CZTSSe thin films selenized at different temperatures

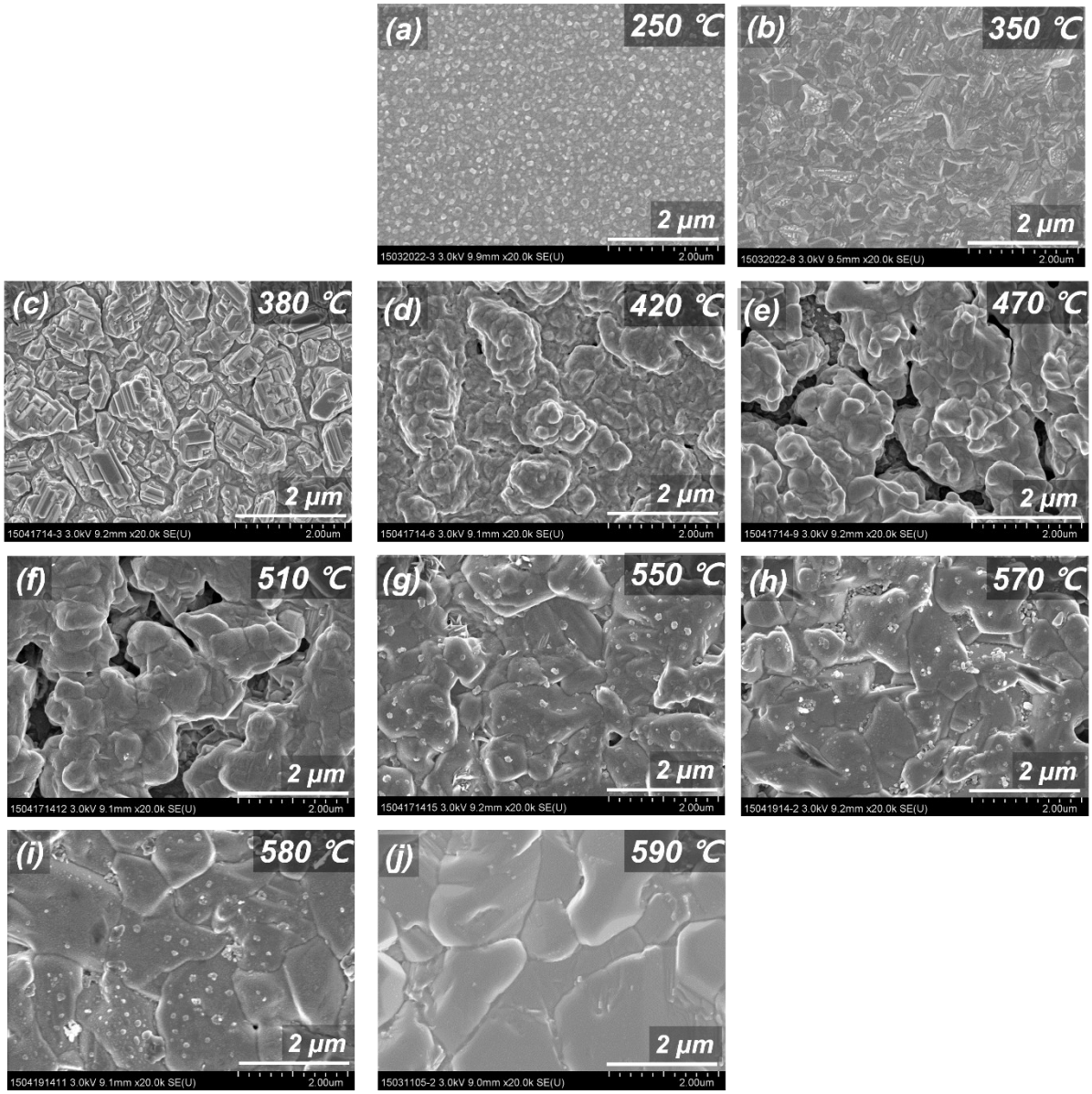

Figure S2. **Figure 4.** Cross-sectional STEM images of the (a) sample cooled after reaching 250 °C, (b) sample cooled after reaching 350 °C, (c) sample cooled after annealing at 380 °C, (d) sample cooled after reaching 420 °C, (e) sample cooled after annealing at 470 °C, (f) sample cooled after annealing at 510 °C, (g) sample cooled after annealing at 550 °C, (h) sample cooled after annealing at 570 °C, (i) sample cooled after annealing at 580 °C and (j) sample cooled after annealing at 590 °C.