Effects of Mo back-contact annealing on surface potential and carrier transport in Cu₂ZnSnS₄ thin film solar cells

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Supplementary materials



Figure S1. Topography of Mo surface with and without annealing. Roughness of each sample is shown above the images. While As-grown and 180 and 370 °C-annealed sample has the roughness of ~ 2.2 nm, 550 °C-annealed sample shows the highest roughness of 4.4 nm, which is double of the others. Na and O diffused from soda lime glass can affect the morphology. Further investigation of this is under way.



Figure S2. SIMS composition profile of annealed Mo back-contact layers. As the annealing temperature is higher, the Na content has been increased in the Mo layers. This affects the growth of the absorber layer.



Figure S3. XPS data indicate the relative concentration of Cu, Zn, Sn, S and Na. The relative concentration of Cu, Zn, Sn and S are relatively consistent as a function of the Mo annealing temperature. (c), however, shows that the Na concentration is increased with the higher Mo annealing temperature. This result suggests that the Mo annealing process encourages Na diffusion into the CZTS absorber layers.



Figure S4. *I-V* curves of the samples were obtained at the GBs and the IG regions in the range of -1.5 V ~ +1.5 V by conductive atomic force microscopy. The local *I-V* characteristics were used to determine the conduction mechanism between the thin film surface and the Pt probe. The *I-V* curves show a position dependence of current on the GBs and IGs. Since the current at the GBs is larger than that at the IG regions, our contact between the probe and the surface is robust. It is difficult to compare the *I-V* curves and deduce an underlying transport mechanism. Detailed work on this is under way.



Figure S5. XRD patterns of Mo back contact layers. (a) is the pattern of annealed Mo back contact sample with nitrogen atmosphere at various temperature and shows Mo peaks. (b) is the pattern of annealed Mo back contact samples after sulfurization process at 570 $^{\circ}$ C.



Figure S6. The data above shows the results of micro-Raman scattering spectroscopy. The measurement is conducted using the laser with wavelength of 488 nm. The scan depth is about 140nm, so we can detect the structure in the CZTS absorber layers. The samples show main CZTS peaks at 287, 336 and 373 cm⁻¹. However, we were not able to find the secondary phase peaks, such as CuS, ZnS and SnS.