Diffusion behaviour of alkali metals after KF-PDT on CIGS thin films fabricated onto sodalime glass substrates

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Introduction

Potassium fluoride post deposition treatment (KF-PDT) is a novel way of incorporation K into CIGS thin films, which improves the conversion efficiency of solar cells [1,2]. In alkali-free substrates, ion-exchange between Na and K has been observed, when KF-PDT was performed after NaF-PDT [1]. However, the effect of KF-PDT on CIGS thin films deposited on SLG substrates may differ from that of alkali-free substrate due to a large amount of K and Na diffused from SLG substrates during growth temperature. In this work, the diffusion behavior of alkali metals has been investigated after KF-PDT on SLG substrates.

Experimental

CIGS thin films $(2.8 \sim 2.9 \mu m)$ were deposited by three-stage process at a maximum substrate temperature of 530°C on Mo-coated SLG substrates. The KF-PDT was performed on CIGS at a substrate temperature of 350°C. XPS measurement was performed using a Quantera scanning XPS microprobe (PHI) with monochromatic Al K α (1.5 keV) X-ray radiation. The depth profiles of the CIGS thin films were obtained by SIMS (PHI ADEPT-1010, Physical Electronics, Chanhassen, MN, USA).

Results and Discussion

Fig 1 shows XPS depth profiles of CIGS thin films fabricated on SLG substrates with and without KF-PDT. As can be seen in this figure, Na atoms outdiffused from the bulk area of CIGS with decreasing Cu atoms after KF-PDT. The diffusion behavior of Na may be due to the migration of Na via V_{Cu} to form Na_{Cu}, This is consistent with the theoretical report in which Na atoms can easily migrate via V_{Cu} whereas K⁺ ions can't easily substitute for Cu⁺ ions due to the larger ionic radius [3]. XPS narrow scan also confirmed that Na segregated as Na-Se binary compounds. The excess Na atoms at the surface region were removed by water-rinsing.

Fig.2 shows SIMS depth profiles of water rinsed CIGS thin films with (solid lines) and without (dotted lines) KF-PDT. In bulk region the Na concentration reduced with increasing K concentration, which could be interpreted as an ionic exchange. In contrast, Na atoms increased at the surface region after KF-PDT, which suggests that the diffusion behaviour of alkali metals on CIGS thin film grown on SLG differs from that grown on alkali-free substrates due to the large supply of Na and K from SLG.



Fig 1 XPS and depth profiles of CIGS thin films with (solid lines) and without (dotted lines) KF-PDT before water rinsing.



Fig 2 SIMS depth profiles of the water rinsed CIGS thin films with (solid lines) and without (dotted lines) KF-PDT.

Conclusion

XPS and SIMS depth profiles suggest that Na atoms were out-diffused at the surface region after KF-PDT of CIGS thin films grown onto SLG substrates, which may be due to migration of Na via V_{Cu} to form Na_{Cu}. The excess Na atoms at the surface region were removed by water-rinsing.

References

[1] Chirila et al., Nature Mater. 12 (2013) 1107-1111.[2] R. Kamada et al., Presented at the IEEE PVSC (2016).

[3] T. Maeda et al., Jap. J. Appl. Phys. 54 (2015) 08KC20(1-8).