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Alkali incorporation into $Cu(In,Ga)Se_2$ determined by crystal orientation of Mo back contact: Implications for highly efficient photovoltaic devices

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ABSTRACT

The structural, optical, and electrical properties of molybdenum (Mo) layers play a major role in $Cu(In,Ga)Se_2$ (CIGS) solar cell performance. The Mo layer works as a transport gate for diffusion of alkali ion from the soda-lime glass substrate to the back contact in CIGS solar cells. In the present work, Mo back contacts are controlled to exhibit two different orientations: (110)-oriented and randomly oriented. The influence of these orientations on CIGS absorbers and resulting solar cells is investigated. *In situ* thermo-Raman spectroscopy and secondary ion mass spectrometry results indicate that the greater amount of alkali ions are found in the CIGS absorber with randomly oriented Mo back contact than in the (110)-orientated Mo back contact. The resulting different Na incorporations significantly affect the performance of the resulting devices. Devices with the randomly oriented Mo back contact exhibit superior device performances to the devices with (110)-oriented Mo back contact. With comprehensive device characterizations, an alkali ion release determined by the orientation of the Mo back contact affects the recombination mechanism in the CIGS bulk and the back contact properties at the CIGS/Mo interface.

1. Introduction

$Cu(In,Ga)Se_2$ (CIGS)-based solar cells are among the most attractive photovoltaic devices owing to their high energy conversion efficiency and competitive fabrication cost [1,2]. Recently, CIGS solar cells have attained high energy conversion efficiencies of over 20% by optimizing fabrication processes such as CIGS composition ratio control or alkali post deposition treatment (PDT) [2]. For higher energy conversion efficiency, large-scale cells/modules, and mass production, quality control of many layers and interfaces are necessary, requiring analysis of basic material properties and electronic loss mechanisms in photovoltaic devices.

Direct current (DC) magnetron sputtered Mo on the soda-lime glass (SLG) is typically employed as the back contact of the CIGS solar cells, owing to its good electrical conductivity and Ohmic contact with the CIGS thin film [3–12]. Mo back contacts have numerous parameters that may affect the characteristics of CIGS solar cells. The effect of the microstructure of Mo back contacts on photovoltaic efficiency has been intensively studied in respect of its effect on the resulting devices [10,13]. Yoon et al. studied the effects of Mo layer microstructure on tensile stress and electrical resistivity [10]. The formation of a $MoSe_2$ layer in the CIGS/Mo interface affects the adhesion of the interface and its contact resistance [6,12,14]. In previous studies, the orientation of the Mo back contact has been found to affect the orientation of the CIGS film, consequently influencing solar cell performance [4,9,15]. Recently, the influence of alkali ions (i.e., sodium or potassium) on the properties of CIGS solar cells has been reported, and how this leads to the enhancement of the solar cell performance [2–4,7,8,11,13,16–19]. Specifically, the properties of Mo back contacts significantly influence the distribution of alkali ions from the SLG substrate [3,4,7,10,11]. Na deficiency in CIGS may degrade the properties of CIGS/Mo junction, causing significant loss of fill factor (*FF*) and open circuit voltage (V_{OC}) [11,20]. However, it is still arguable that how highly a Mo back contact affects the alkali ions' diffusion in the CIGS absorber and consequently the resulting devices. Thus, new directional and comprehensive analyses are needed, to elucidate the abovementioned questions and to further improve CIGS solar cell performance.

Thermo-Raman spectroscopy is convenient for providing information on the in situ investigation of composition changes [21]. This technique can evaluate the alkali ion diffusion changes with increasing

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