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Characterization of TiN back contact interlayers with varied thickness for $Cu_2ZnSn(S,Se)_4$ thin film solar cells

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Abstract

TiN thin films have previously been used as intermediate barrier layers on Mo back contacts in CZTS(e) solar cells to suppress excessive reaction of the Mo in the annealing step. In this work, TiN films with various thickness (20, 50 and 200 nm) were prepared with reactive DC magnetron sputtering on Mo/SLG substrates and annealed, without CZTS(e) layers, in either S or Se atmospheres. The as-deposited references and the annealed samples were characterized with X-ray Photoelectron Spectroscopy, X-ray Diffraction, Time-of-Flight-Elastic Recoil Detection Analysis, Time-of-Flight-Medium-Energy Ion Scattering, Scanning Electron Microscopy and Scanning Transmission Electron Microscopy – Electron Energy Loss Spectroscopy. It was found that the as-deposited TiN layers below 50 nm show discontinuities, which could be related to the surface roughness of the Mo. Upon annealing, TiN layers dramatically reduced the formation of $MoS(e)_2$, but did not prevent the sulfurization or selenization of Mo. The $MoS(e)_2$ had formed near the discontinuities, both below and above the TiN layers. Another unexpected finding was that the thicker TiN layer increased the amount of Na diffused to the surface after anneal, and we suggest that this effect is related to the Na affinity of the TiN layers and the $MoS(e)_2$ thickness.