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Technology for Si/CZTS Tandem Solar Cell

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Photovoltaic (PV) technology, that directly converts the abundant solar photons into electrical energy, has developed into one of the most promising sustainable energy technologies due to continued reductions in costs. Single material solar cells, however, are now as efficient as physical and practical limits allow. To improve efficiency further, tandem (or multi-junction) solar cells with complementary band gaps must be used, since this approach allows efficiency beyond the “detailed balance” limit for single junction solar cells\textsuperscript{1} due to reduced thermalization losses\textsuperscript{2}.

Silicon-based tandem solar cells have attracted huge attention over the recent years as they can leverage the well-established manufacturing capacity of the existing crystalline silicon technologies. A suitable, i.e., inexpensive, earth abundant, stable and non-toxic, material with an appropriate bandgap to be used as the top cell absorber has, however, yet to be identified. CZTS, a quaternary compound semiconductor based on non-toxic and earth abundant elements (Cu\textsubscript{2}ZnSnS\textsubscript{4}), with a band gap of 1.5 eV, is a promising candidate for the upper cell\textsuperscript{3}. However, integrating CZTS with silicon is challenging due to silicon-incompatible processing steps in synthesis of CZTS, such as high temperature (550-600°C) annealing of the metallic precursors in a sulfur atmosphere. This can lead to inter-diffusion of detrimental metallic elements (e.g., Cu) into the bottom silicon cell. Since silicon is sensitive to metallic contamination, this may result in extremely poor performance of the device. Therefore, developing a tunnel/barrier layer between the two absorbers will be a decisive innovation for the construction of such a cell.

Here, we present an initial evaluation of titanium nitride (TiN) as a potential material for the tunnel/barrier layer\textsuperscript{4}. Optical simulations using the net-radiation method\textsuperscript{5} were performed on a simplified tandem structure to estimate the optical performance of TiN as the buffer layer. It was established that at most 15-20 nm of TiN can be tolerated before the optical losses due to absorption in TiN is significant. The diffusion barrier properties of TiN deposited with Plasma Enhanced Atomic Layer Deposition (PEALD) were investigated using a simple stack of Si/TiN(25nm)/Cu, which was isothermally annealed in vacuum at 550°C to simulate the CZTS synthesis conditions. After the annealing, the samples were characterized by X-Ray diffraction (XRD), four point probe measurements, and X-Ray Photoelectron Spectroscopy (XPS) to determine the effectiveness of the TiN diffusion barrier. It was concluded that 25 nm of TiN was not enough to avoid Cu in-diffusion to the Si layer, as revealed by the presence of Copper Silicides (Cu\textsubscript{2}Si) from XRD analysis and an increased sheet resistance inherent to these Cu compounds.