

Structural and Compositional Properties of Recrystallized CdS/CdTe Thin-Films Grown on Oxidized Silicon Substrates

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Cadmium telluride (CdTe) thin-films are the most promising photovoltaic (PV) materials for lightweight and flexible solar cells because of their excellent light absorption (i.e., direct band-gap of 1.45 eV) and low-cost manufacturing processes. To improve the specific power (kW kg^{-1}) and mechanical flexibility, recent research has focused on new PV design and low-temperature ($< 450\text{ }^\circ\text{C}$) deposition processes, where the active *n*-CdS/*p*-CdTe layers are directly deposited on lightweight substrates, such as polymer [1, 2] and metal foils [3]. However, the measured PV efficiencies of these low-temperature devices ($< 14\%$) are still far below than those fabricated using high-temperature processing methods ($> 22\%$). Recognizing this temperature disparity, our approach is based on high-temperature CdTe synthesis ($> 450\text{ }^\circ\text{C}$) on an oxidized silicon wafer (Si/SiO₂) that can decouple the high-temperature grain growth and the subsequent thin-film lift-off / transfer processes (Figure 1). This method enables the integration of the high-quality CdS/CdTe active layers on lightweight and flexible substrates (e.g., plastic, fabric, cellulose paper) that have having the limited temperature tolerance.

In this work, we apply the post-annealing CdCl₂ treatments that are frequently used for conventional CdTe PVs fabricated on fluorine-doped tin oxide (FTO). Several previous work reported that this CdCl₂ treatments radically increase the CdTe grain size and also enhance their local optoelectronics properties. [4-6]. Prior to CdTe deposition, a thin-layer of CdS (200 nm) was evaporated at room temperature on Si/SiO₂ substrates. A 4 μm thick CdTe layer was then thermally evaporated at a fixed substrate temperature of 300 $^\circ\text{C}$, 400 $^\circ\text{C}$, 450 $^\circ\text{C}$, and 500 $^\circ\text{C}$, respectively. A portion of each sample was cleaved off and placed upside down in a graphite boat filled with CdCl₂ pellets in a tube furnace. The samples were annealed at 410 $^\circ\text{C}$ for 15 minutes in N₂. Figure 2 summarizes the CdTe grain size before and after the post-annealing treatments. The nominal grain size of the treated CdTe film reaches to approximately 7 μm for all samples extracted using the MIPAR software (Materials Image Processing and Automated Reconstruction) [7]. Overall, the CdTe grain size of our samples is much larger than those in conventional CdTe solar cells on glass/FTO (typical size of $\approx 1\text{ }\mu\text{m}$). The small voids near grain boundaries are noticeable with the CdCl₂ treated CdTe sample at 300 $^\circ\text{C}$ (Figure 2c) than in the 500 $^\circ\text{C}$ sample (Figure 2e). Presumably, these voids were introduced by the physical expansion of small grains (100 nm) to large ones (7 μm) during the grain recrystallization. Figure 3 shows the scanning transmission electron microscopy (STEM) and simultaneously collected energy-dispersive x-ray spectroscopy (EDX) collected by high-resolution dual detectors, confirming that highly uniform compositions of CdS and CdTe layers, closely resembling the intended configuration. Interestingly, the Te-*L* map reveals a distinct Te layer at the interface of CdS and SiO₂ (Figure 3d) that has not been seen in conventional CdS/CdTe PVs on FTO. We believe that the presence of this 20 nm Te-rich layer would promote the delamination of as-grown CdS/CdTe films from Si/SiO₂ substrate in water, similar to the lift-off of flexible electronics based on Ni films [8]. This Te-rich region was disappeared under the CdCl₂ treatments (Figure 3f), and it is rather uniformly redistributed in the CdS film as seen in

quantitative EDX linescans. The CdCl_2 treated samples can also be lifted-off in water like as-grown CdS/CdTe samples. The underlying physical mechanisms responsible for the delamination of as-grown and CdCl_2 -treated CdS/CdTe samples are under investigation.

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