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Photovoltaic optimization of SILAR-deposited cadmium telluride nanocrystals for semiconductor-sensitized solar cells

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Abstract. Cadmium telluride (CdTe) is one of the most promising materials for photovoltaic applications due to its nearly optimal band gap of 1.45 eV and strong optical absorption capability. This work aimed to synthesize CdTe using the successive ionic layer adsorption and reaction (SILAR) method and to optimize the SILAR conditions for producing efficient CdTe nanocrystals (NCs) as sensitizers in semiconductor-sensitized solar cells (SSCs). The optimization process involves evaluating the effects of varying tellurium precursor solutions, annealing durations, the number of SILAR cycles, and Cd solution dipping times on the photovoltaic performance of CdTe NC-SSCs. The results indicated that the optimal photovoltaic performance of CdTe NC-SSCs fabricated via the SILAR method was achieved using a tellurium precursor solution composed of tellurium powder, DI water, and sodium borohydride, an annealing duration of 20 minutes at 400°C, five SILAR cycles, and a Cd dipping time of 90 seconds. X-ray diffraction (XRD) analysis confirmed the cubic crystal structure of the synthesized CdTe with an average particle size of 19.47 nm. The best power conversion efficiency (PCE) achieved was 1.28% (J_{sc} of 5.85 mA/cm^2, V_{oc} of 0.44 V, and FF of 49.80%). These findings demonstrate the viability of CdTe NCs synthesized by the SILAR method as effective sensitizers in SSCs. The obtained efficiency of 1.28% represents the highest PCE reported for pure CdTe via SILAR to date, suggesting that further optimization and interface engineering could lead to even greater performance improvements.

1. Introduction

Cadmium Telluride (CdTe) is a II–VI semiconductor with excellent potential as a light absorber in semiconductor-sensitized solar cells (SSCs), offering properties that align well with the development of more responsible, future-oriented photovoltaic technologies. It possesses an ideal band gap of approximately 1.45 eV. It exhibits suitable band alignment with metal oxides such as TiO_2, forming a type-II staggered band interface that facilitates efficient charge separation and

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transfer. Additionally, CdTe has a high optical absorption coefficient of approximately 10^4 cm^{-1}[1,2]. Despite these advantages, the power conversion efficiency (PCE) of CdTe-based SSCs remains lower than that of other II–VI quantum dot sensitizers, such as CdS and CdSe. CdS, with a wider bandgap of approximately 2.4 eV, has achieved PCE values of up to 3.7%[3], while CdSe-based devices have reported PCEs as high as 6.7%[4]. In contrast, CdTe-based SSCs have only sporadically reached higher PCEs, with a maximum reported value of approximately 4.87% under optimized aqueous-based deposition conditions[5]. Nevertheless, most CdTe-based SSCs exhibit PCEs below 1%, indicating that high performance in this system remains difficult to achieve reproducibly [6–8]. This limitation is primarily due to its poor electrochemical stability and severe charge recombination caused by intrinsic defects [9]. To address these challenges, researchers have explored strategies such as applying passivation layers or engineering core/shell structures. For instance, incorporating a ZnS passivation layer [6,8] or forming CdTe/CdS core/shell structures [7,10] has shown promise in improving performance.

Nonetheless, employing CdTe as the sole light absorber in SSCs remains a considerable challenge. To address this, the fabrication method must also be practical and cost-effective to support wider adoption. Various synthesis techniques have been explored for producing CdTe-based SSCs, including the chemical reduction method[8], aqueous colloidal chemical synthesis[6], hydrothermal method[7], linker-assisted (LA) method [11], linker-assisted chemical bath deposition[10], and aqueous synthesis route[5]. Despite their effectiveness, these approaches suffer from notable limitations: hydrothermal synthesis requires high temperatures, high pressures, and long reaction times, which complicate scalability, while LA and LACBD rely on organic linkers that can introduce interfacial resistance and increase fabrication complexity. Moreover, aqueous synthesis routes achieving relatively high efficiencies (e.g., 4.87% [5]) typically demand tightly controlled, multistep processes, potentially limiting reproducibility and practical implementation. In comparison with the aforementioned synthesis methods, successive ionic layer adsorption and reaction (SILAR) offers several advantages: it enables precise control over morphology and particle size through cycle regulation, operates under ambient conditions, and does not require high-purity target materials [12]and allows in situ growth on the TiO_2 surface, potentially enhancing charge transfer and interfacial stability[13]. To the best of our knowledge, the SILAR technique has not yet been systematically employed to fabricate CdTe-based SSCs with a reasonable PCE.

Building on the previous discussion, this study focuses on the synthesis of CdTe nanocrystals (NCs) via the SILAR technique, aiming to optimize deposition parameters to enhance their performance as sensitizers in SSCs. The structural characteristics of the resulting CdTe NCs were investigated using X-ray diffraction (XRD). Photovoltaic performance was systematically evaluated by varying the tellurium (Te) precursor composition, annealing time, number of SILAR cycles, and cadmium (Cd) dipping duration. Through this optimization process, the devices achieved a PCE representing the highest reported value for CdTe NC-based SSCs fabricated using the SILAR method. These findings represent a significant advancement in the development of cost-effective CdTe sensitizers and contribute to broader efforts to rationalize the design of efficient and sustainable photovoltaic technologies.

2. Experimental section

Unless otherwise specified, all reagents and materials were used as received without additional purification. Detailed experimental procedures are described in the following subsections.

2.1. TiO_2 photoanode preparation

A three-layer TiO_2 photoanode architecture was employed in this work and deposited onto fluorine-doped tin oxide (FTO) glass substrates (7 Ω/sq, Ruilong, Taiwan) [14–16]. The compact TiO_2 blocking layer, with a thickness of approximately 50–70 nm, was formed by spin-coating 50 μL of a 0.247 M titanium(IV) isopropoxide (Sigma-Aldrich, 97%) precursor solution onto thoroughly cleaned FTO substrates. Subsequently, a mesoporous TiO_2 film (mp-TiO_2) with an average thickness of ~10–12 μm and particle size of around 30 nm was deposited using the doctor-blade technique with a commercial DSL 30NR-T paste (GreatCell Solar), followed by drying at 120 °C for 5 minutes. To enhance light scattering, an additional TiO_2 overlayer containing larger particles (300–400 nm) with a thickness of approximately 5 μm was applied using a WER2-O paste (GreatCell Solar). The assembled photoanode structure was finally sintered at 500 °C for 90 minutes to ensure film adhesion and crystallinity [17].

2.2. CdTe nanocrystals (NCs) synthesis procedure

CdTe NCs were grown directly on TiO_2 photoanodes via a successive ionic layer adsorption and reaction (SILAR) process. In a typical deposition sequence, the TiO_2 electrodes were alternately exposed to cadmium and tellurium precursor solutions to form CdTe nanocrystals on the TiO_2 surface. Cadmium incorporation was achieved by immersing the photoanodes in a 0.1 M cadmium acetate (Alfa Aesar, 98%) solution prepared in methanol for 60, 90, or 120 s, followed by rinsing with methanol and drying at 40°C. The electrodes were subsequently treated with a tellurium precursor solution for 60 s, rinsed with ethanol, and dried under the same conditions.

One complete CdTe deposition cycle consisted of successive cadmium and tellurium treatments, and the procedure was repeated three to five times to control the surface loading of CdTe NCs. Post-deposition thermal treatment was performed at 400°C under ambient conditions for different annealing durations (10, 10–20, and 15–15 min) to improve interfacial contact and crystallinity.

Two types of tellurium precursor solutions were investigated for comparison: (i) 0.16 M Na_2TeO_3 (Sigma-Aldrich, 99%) dissolved in deionized water with sodium borohydride (Alfa Aesar, 98%) as the reducing agent, and (ii) 0.7 mM tellurium powder (Thermo Scientific Chemicals, 99.99%) dispersed in deionized water with sodium borohydride.

2.3. Device assembly and characterization techniques

Liquid-junction CdTe nanocrystal-sensitized solar cells (NC-SSCs) were fabricated by combining CdTe-modified TiO_2 photoanodes with CuS counter electrodes, separated by a parafilm spacer with a thickness of approximately 190 μm. The CuS counter electrodes were prepared via a chemical bath deposition (CBD) method following established procedures [15]. Prior to electrical characterization, a polysulfide-based electrolyte was introduced into the inter-electrode space to complete the cell configuration. The structural properties of the fabricated devices were examined using X-ray diffraction (XRD) (Bruker D8), while their photovoltaic performance was evaluated through current density–voltage (J–V) measurements (Keithley 2400 source meter under 100 mW/cm^2 light illumination from a 150 W Xe lamp). All characterization procedures were conducted in accordance with previously reported methodologies [4,18].

3. Results and discussions

3.1. Analysis of CdTe nanocrystal structure

The crystalline structure of the synthesized CdTe nanocrystals (NCs) was analyzed using X-ray diffraction (XRD). As shown in Figure 1, the diffraction peaks are consistent with the cubic phase of CdTe (JCPDS No. 03-065-8395), with no detectable impurities. Prominent peaks were observed

at (111) at 2θ = 23.75°, (220) at 2θ = 39.28°, and (311) at 2θ = 46.42°. Some studies have reported that the SILAR method consistently yields a cubic CdTe phase, despite variations in precursor concentration and chemical composition [13,19,20]. In addition, peaks corresponding to TiO_2 (JCPDS No. 01-071-1169) and SnO_2 (JCPDS No. 00-046-1088) were also present in the XRD pattern, as the CdTe NCs were directly grown within the mesoporous TiO_2 (mp-TiO_2) matrix on FTO glass via *in situ* synthesis.

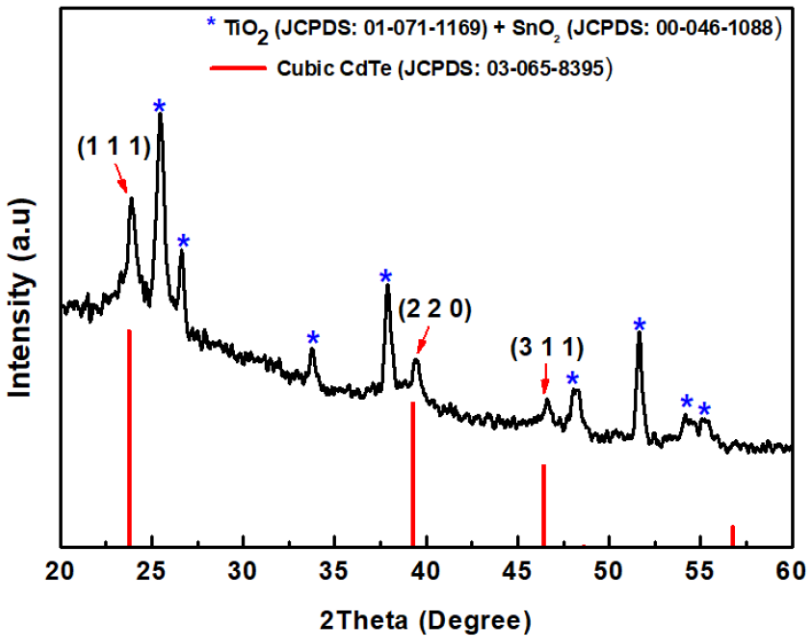


Figure 1. XRD pattern of the prepared CdTe NCs

The lattice parameters for the synthesized CdTe NCs were calculated using equations (1) and (2) from those three peaks.

$$n\lambda = 2d \sin\theta \quad (1)$$

$$\frac{1}{d^2} = (h^2 + k^2 + l^2)\frac{1}{a^2} \quad (2)$$

where λ equal to 1.5406 Å. The results are $a = b = c$ = 6.470 Å, which is slightly different from the bulk cubic CdTe of 6.482 Å.

By using the Scherrer equation (equation (3)) from three peaks,

$$D = \frac{K\lambda}{\beta \cos\theta} \quad (3)$$

In which λ = 1.5406 Å, and the shape vector K=9, the crystallite size D was (i) 16.15 nm for the (111) peak, (ii) 14.34 nm for the (220) peak, and (iii) 27.93 nm for the (311) peak, resulting in the average crystallite size of CdTe NCs of 19.47 nm. Smaller particle sizes (8–12 nm) have been reported in other studies [16,17], which may be attributed to differences in kinetic parameters such as precursor concentration, adsorption time, number of cycles, and annealing conditions, as these factors influence nucleation and growth processes and ultimately affect particle size.

3.2. Analysis of photovoltaic performance under different tellurium (Te) precursor solutions

The photovoltaic characteristics of liquid-junction CdTe NC-SSCs were systematically evaluated for devices fabricated using different Te precursor solutions. The extracted photovoltaic parameters—namely the short-circuit current density (J_{sc}), open-circuit voltage (V_{oc}), fill factor (FF), and PCE—are compiled in Table 1, while the corresponding *J–V* characteristics are presented in Figure 2.

Table 1. Photovoltaic performance of CdTe NC-SSCs under different Te precursor solutions.

Te Precursor Solution	J_{sc}(mA cm^{-2})	V_{oc}(V)	FF(%)	PCE(%)
Na_2TeO_3/Deionized water	3.18	0.40	39.17	0.498
Te Powder/Deionized water	3.77	0.42	56.94	0.901

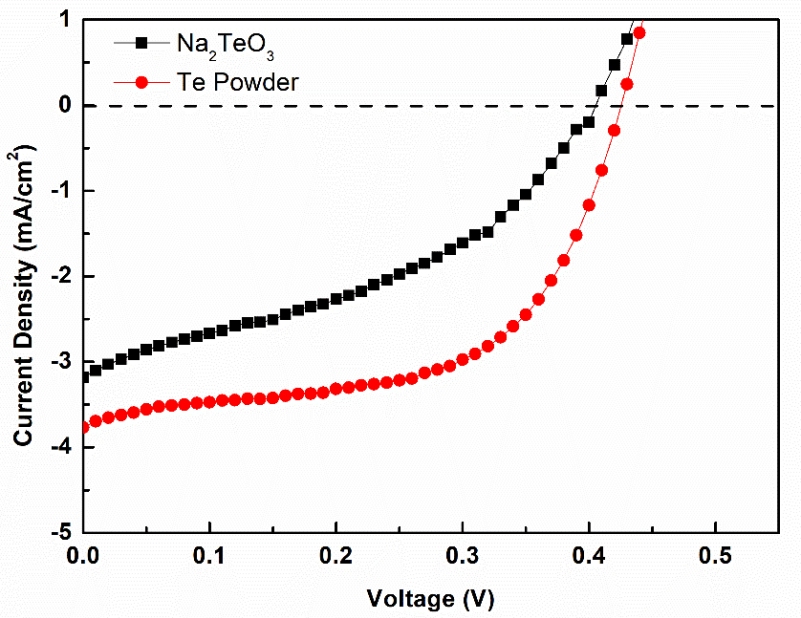


Figure 2. *J-V* curve of CdTe NC-SSCs under different Te precursor solutions

Among the investigated systems, devices prepared using a Te powder–based precursor dissolved in deionized water exhibited superior photovoltaic performance compared with those fabricated from Na_2TeO_3-derived precursors. The optimized device delivered a PCE of 0.901%, together with a J_{sc} of 3.77 mA cm^{-2}, a V_{oc} of 0.42 V, and an FF of 56.94%. This improvement is attributed to the more direct control of Cd: Te stoichiometry afforded by the Te powder precursor, thereby avoiding the introduction of sodium-related species. In contrast, Na_2TeO_3-based solutions inherently contain Na^+ ions that may be incorporated into the CdTe lattice or segregate at grain boundaries, leading to degraded crystallinity and compromised device performance, resulting in only the PCE of 0.498% (J_{sc}=3.18 mA cm^{-2}, V_{oc}=0.40 V, FF=39.17%). Similar observations have been reported in the literature. Nideep *et al.* fabricated CdTe QDSSCs using an aqueous chemical reduction method with Na_2TeO_3 as the tellurium source and achieved a PCE of 0.53%[6]. In contrast, Amani-Ghadim *et al.* employed Te powder as the precursor in a

hydrothermal deposition method, resulting in a higher efficiency of 0.71%[7]. Although the fabrication methods differ, these findings indicate that Te powder–based precursor systems may offer advantages for CdTe formation, including in SILAR-based and related deposition approaches. The results also show that the PCE of 0.901% produced by the SILAR method can be more efficient than those obtained using the aforementioned methods.

3.3. Analysis of photovoltaic performance under different annealing durations

The photovoltaic performance of liquid-junction CdTe NC-SSCs was further evaluated under varying annealing durations at 400°C. Table 2 presents the corresponding photovoltaic parameters, while the *J–V* characteristics for each condition are illustrated in Figure 3.

Table 2. Photovoltaic performance of CdTe NC-SSCs under different annealing durations.

Annealing Duration (at 400°C)	J_{sc}(mA cm^{-2})	V_{oc}(V)	FF(%)	PCE(%)
10 min; 10 min	1.21	0.27	28.55	0.0931
10 min; 20 min	3.82	0.39	56.98	0.848
15 min; 15 min	3.18	0.40	39.17	0.498

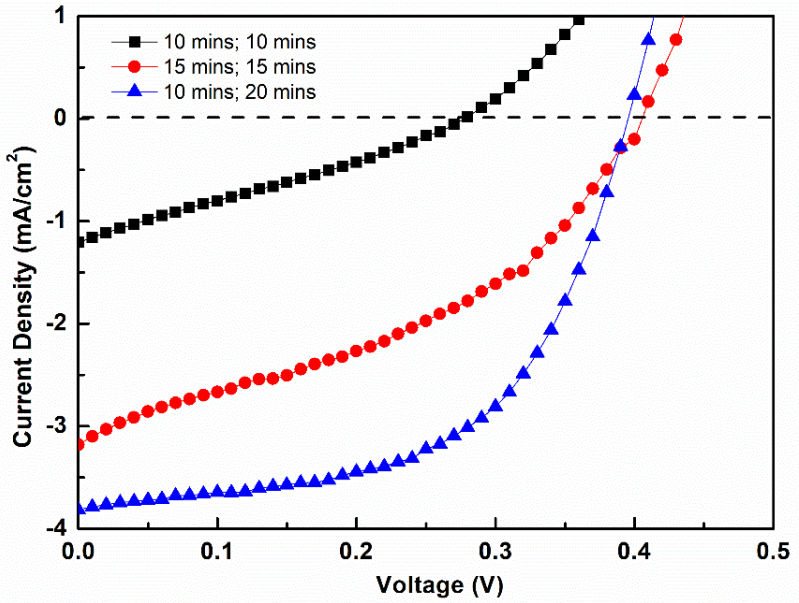


Figure 3. *J-V* curve of CdTe NC-SSCs under different annealing durations

As shown in Table 2, an annealing sequence of 10 minutes at the temperature ramping stage and 10 minutes at the annealing stage resulted in only 0.0931% (J_{sc}=1.21 mA cm^{-2}, V_{oc}=0.27 V, FF=28.55%), indicating that insufficient annealing duration leads to poor crystal growth and inadequate interfacial contact between the CdTe NCs and the mp-TiO_2, generating defect states that act as charge recombination centers[21,22]. A further increase in the annealing stage duration to 20 minutes (10 min; 20 min data) produced the highest device efficiency, yielding a PCE of 0.848%, with a J_{sc} of 3.82 mA cm^{-2}, a V_{oc} of 0.39 V, and an FF of 56.98%. This improvement is attributed to optimized thermal treatment, which promotes enhanced crystallinity and grain growth in the CdTe layer. As a result, the density of grain-boundary traps is reduced, allowing charge carriers to have improved transport. The annealing process provides sufficient thermal

energy to facilitate crystal reorganization and defect passivation, thereby boosting charge collection efficiency and overall device performance [21–23]. However, a higher temperature ramping stage duration of 15 minutes did not improve the performance (PCE=0.498%, J_{sc}=3.18 mA cm^{-2}, V_{oc}=0.40 V, FF=39.17%). This suggests that extending the temperature ramping stage alone, without a corresponding increase in the annealing duration, is insufficient, indicating that the annealing stage plays a more critical role in promoting crystal growth of CdTe NCs than the ramping process.

3.4. Analysis of photovoltaic performance under different SILAR cycles

Under the optimized conditions previously established—using Te powder as the precursor and annealing for 10 minutes, followed by an additional 20 minutes at 400°C—the photovoltaic behavior of Te NC-SSCs was systematically examined as a function of SILAR deposition cycles, ranging from 3 to 5. The extracted photovoltaic parameters are presented in Table 3, while the corresponding *J–V* curves are shown in Figure 4.

Table 3. Photovoltaic performance of CdTe NC-SSCs under different SILAR cycles.

SILAR Cycles	J_{sc}(mA cm^{-2})	V_{oc}(V)	FF(%)	PCE(%)
3	3.55	0.38	47.67	0.643
4	3.71	0.41	56.28	0.857
5	3.77	0.42	56.94	0.901

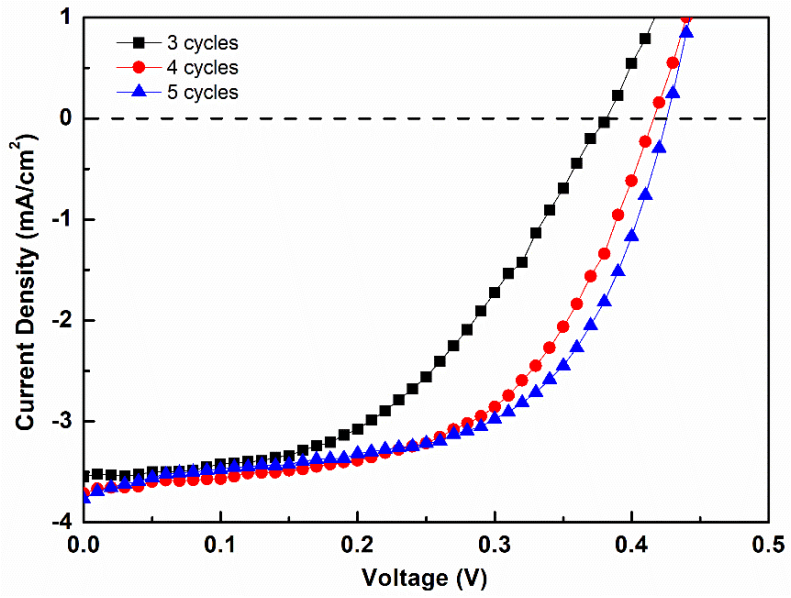


Figure 4. *J-V* curve of CdTe NC-SSCs under different SILAR cycles

Based on Table 3, three SILAR cycles resulted in the PCE of 0.643% (J_{sc}=3.55 mA cm^{-2}, V_{oc}=0.38 V, FF=47.67%). Increasing the number of SILAR cycles to four improved the PCE to 0.857%, with a J_{sc} of 3.71 mA cm^{-2}, a V_{oc} of 0.41 V, and an FF of 56.28%. Furthermore, the cell fabricated with five SILAR cycles delivered the best performance, yielding a power conversion efficiency of 0.910%, together with a J_{sc} of 3.77 mA cm^{-2}, a V_{oc} of 0.42 V, and an FF of 56.94%. This performance enhancement is mainly ascribed to the increased number of SILAR cycles, which

promotes the growth of larger CdTe NCs, enabling stronger light absorption and consequently higher photocurrent generation. Similar trends were also observed in other binary materials within the same group, such as CdS QDSSCs [24] and CdSe QDSSCs [4]. As noted in our previous study, the number of SILAR cycles plays a crucial role in determining PCE [25].

3.5. Analysis of photovoltaic performance under different cadmium (Cd) dipping times

After establishing the optimal condition for the SILAR process, the Cd dipping time was further investigated to determine whether device performance could be enhanced. Building on the previously identified best result of five SILAR cycles, the Cd dipping duration was varied among 60, 90, and 120 seconds. The photovoltaic parameters are listed in Table 4, while the *J–V* curves are shown in Figure 5.

Table 4. Photovoltaic performance of CdTe NC-SSCs under different Cd dipping times.

Cd Dipping Time (s)	J_{sc}(mA cm^{-2})	V_{oc}(V)	FF(%)	PCE(%)
60	3.77	0.42	56.94	0.901
90	5.85	0.44	49.80	1.28
120	5.94	0.47	36.89	1.03

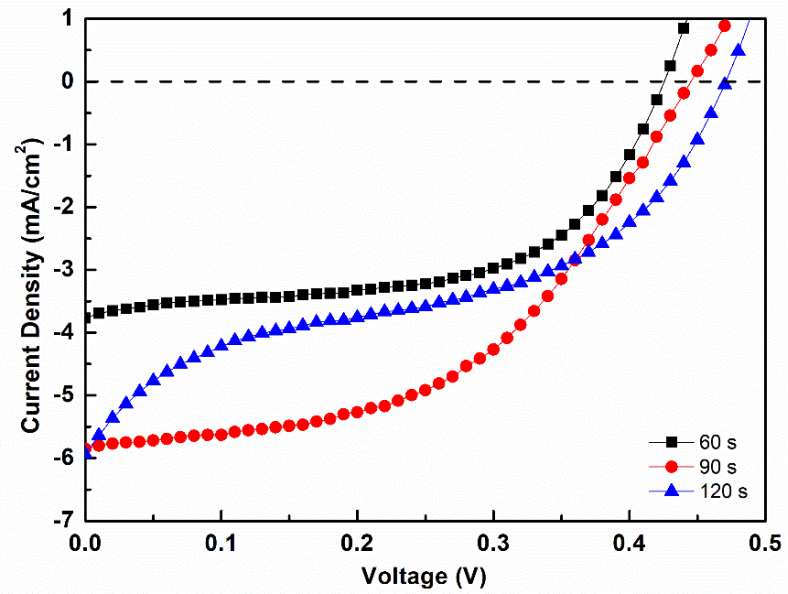


Figure 5. *J-V* curve of CdTe NC-SSCs under different Cd dipping times

Table 4 shows that 60 seconds of dipping time produced the PCE of 0.901% (J_{sc}=3.77 mA cm^{-2}, V_{oc}=0.42 V, FF=56.94%). Further increase of Cd dipping time to 90 seconds, yielding the highest PCE of 1.28%, along with a J_{sc} of 5.85 mA/cm^2, a V_{oc} of 0.44 V, and a FF of 49.80%. Extended Cd dipping times enable greater Cd deposition, which improves absorber layer coverage and enhances light absorption, leading to increased photogenerated current. Additionally, the slight improvement in V_{oc} observed with longer dipping durations may be attributed to a reduction in interface defect density [24,26]. However, excessive dipping, such as the 120-second condition,

can lead to the formation of interfacial residues that hinder charge transport. This manifests as a "rounded" *J–V* curve near the maximum power point, ultimately reducing the FF and overall device efficiency (PCE=1.03%, J_{sc}=5.94 mA cm^{-2}, V_{oc}=0.47 V, FF=36.89%). To date, the CdTe NC-SSCs fabricated in this study have achieved a PCE of 1.28%, which represents the highest reported value for CdTe NC-SSCs prepared using the SILAR method.

The results of this study indicate that the SILAR method for fabricating CdTe-based SSCs has significant potential as a cost-effective alternative to more complex deposition techniques, offering advantages for future commercialization and reduced environmental impact. The SILAR process operates at relatively low temperatures, requires simple equipment, and minimizes material waste, thereby lowering fabrication costs and energy consumption. Furthermore, the controlled use of precursor concentrations and optimized annealing conditions can help limit excessive cadmium consumption, mitigating environmental concerns associated with toxic heavy metals. Collectively, these advantages suggest that CdTe NC-SSCs prepared using optimized SILAR parameters are promising candidates for scalable, low-cost photovoltaic manufacturing with reduced environmental impact.

4. Conclusion

Efficient CdTe nanocrystal-sensitized solar cells (CdTe NC-SSCs) were successfully fabricated using a facile SILAR technique. X-ray diffraction (XRD) analysis confirmed that the synthesized CdTe nanocrystals possess a cubic crystal structure with an average particle size of 19.74 nm. The devices demonstrated optimal photovoltaic performance after five SILAR cycles, achieving a power conversion efficiency (PCE) of 1.28%, the highest reported to date for pure CdTe NC-SSCs prepared via the SILAR method. These findings indicate that SILAR-based CdTe SSCs hold promise for cost-effective and scalable fabrication, provided that process reproducibility and material utilization efficiency are carefully addressed. Future studies should focus on optimizing cell architecture to improve long-term device stability.

Acknowledgments

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