Supporting information Influence of substrate bias and post-deposition Cl treatment on CdTe film grown by RF magnetron sputtering for solar cells

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Experiment:

SnO₂:F –coated soda-lime glass (TEC15) provided by NSG-Pilkington are used as substrates in this study. 5Ns CdTe powder were purchased from a proprietary Chinese supplier and home compressed by hot compression in an inert gas ambiance. During all the deposition, target-substrate distance was kept at 11 cm for all film depositions. 100-130 nm CdS window layer was deposited by RF magnetron sputtering with substrate temperature of 250 °C, argon gas flow rate of 40 sccm, 2 Pa pressure and RF power density of 0.88 W/cm² prior to all the CdTe deposition in this study. The 2-2.3 μ m CdTe thin film was deposited on the top of as-grown CdS without vacuum break. The sputtering condition was as following: substrate temperature of 250 °C, argon gas flow rate of 40 sccm, 2 Pa pressure and RF power density of 0.88 Cm² prior to all the CdTe deposition in this study. The 2-2.3 μ m CdTe thin film was deposited on the top of as-grown CdS without vacuum break. The sputtering condition was as following: substrate temperature of 250 °C, argon gas flow rate of 40 sccm, 2 Pa pressure and RF power density of 1.32 W/cm². The thickness of CdS and CdTe was monitored by an in-situ optical thickness control system. In addition to these, CdTe films were RF sputtered onto the TEC15/

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SnO₂/CdS substrates with floating voltage and different substrate DC bias. The biases were applied through a vacuum feed-through. When 0 V DC bias was applied, TCO of the substrate was grounded to the chamber wall. Thickness of CdTe thin-films with different substrate bias were kept to 2-2.3 μ m. Film growth rate decreases with more negative substrate bias when the RF power density was kept constant. A post-deposition CdCl₂ treatment was carried out at 400 °C for 43 min in a dry air atmosphere. During the treatment, the CdTe films were kept at 1~2 mm away above a CdCl₂ source layer in a glass enclosed space. After CdCl₂ annealing treatment, the remaining CdCl₂ on the surface of CdTe thin-film was rinsed by methanol. Then Cu/Au back contacts in circular shape with thickness of 4/25 nm and radius of 3 mm was evaporated on to the CdTe surface, followed by a thermal activation process at 170 °C for 40 min.



Figure S1. Detailed apparatus diagram of thickness monitoring system

Film thickness thickness monitoring system:

In our system, during CdS growth, a laser with 408 nm was used as the optical resource. While for CdTe, a laser with 633 nm was used as the optical resource. For in-situ CdS thickness measurement, the substrate was firstly heated to the growth temperature, then the laser was open. At this time, the current was measured and regarded as I_0 . During CdS growth, the substrate temperature was kept at constant. I was measured and recorded by our in-situ thickness software, the thickness can be calculated according to the equation: $I = I_0 e^{-\alpha d}$, where α is abortion coefficient, d is the thickness. The thickness was then corrected by step apparatus. Then we can obtain α according to the equation: $I = I_0 e^{-\alpha d}$. The thickness of the obtained film can be in-situ measured based on the obtained α value. For in-situ CdTe thickness measure, the substrate coated with CdS was kept at the growth temperature. Before the CdTe

growth, the current was measured and regarded as I_0 . The in-situ thickness measurement procedure was as the same to that for CdS films.

Table S1. Influence of deposition pressure on mean free path (MFP) and average probability of collision (APC) for sputtered atoms and ions. The APC is equal to 118 mm/MFP

| | Mean free path (mm) | | | | Average probability of collision | | | |
|-----------------------|---------------------|--------|--------|--------|----------------------------------|--------|--------|--------|
| Ion/atom | | | | | (APC) | | | |
| | 4.0 Pa | 3.0 Pa | 2.0 Pa | 1.5 Pa | 4.0 Pa | 3.0 Pa | 2.0 Pa | 1.5 Pa |
| Ar^+ | 11.6 | 15.4 | 23.1 | 30.8 | 10.20 | 7.65 | 5.10 | 3.83 |
| S | 8.4 | 11.2 | 16.8 | 22.4 | 14.05 | 10.53 | 7.02 | 5.27 |
| Cd | 3.4 | 4.6 | 6.9 | 9.1 | 34.43 | 25.82 | 17.22 | 12.91 |
| Te | 3.6 | 4.8 | 7.2 | 9.6 | 32.62 | 24.46 | 16.31 | 12.23 |
| Te ₂ | 1.6 | 2.1 | 3.2 | 4.2 | 74.61 | 55.96 | 37.31 | 27.98 |



Fig. S2. Dependence of (a) E_{ff} (b) Voc (c) Jsc (d) FF for CdTe solar cells as a function of Cl treatment temperature.

Table S2 The highest efficiency of CdTe solar cells with CdTe deposited at different temperature

| | 250 °C | 260 °C | 270 °C |
|---------------------------|--------|--------|--------|
| Voc (V) | 0.759 | 0.744 | 0.772 |
| Jsc (mA/cm ²) | 22.9 | 23.34 | 21.22 |
| FF | 69.03 | 65.19 | 67.81 |
| Eff | 12.00 | 10.85 | 10.91 |