Passivating ion defects on the surface of perovskite films through organic amine compounds reduces the degradation mechanism of perovskite solar cells

Abstract

In recent years, perovskite solar cells have been recognized as one of the most promising types of solar cells due to their tunable bandgap, long exciton diffusion length, and high charge carrier mobility. Despite the rapid improvement in the power conversion efficiency (PCE) of perovskite solar cells, device stability remains a challenge. We have discovered that ion defects, particularly vacancies and under-coordinated lead ions, lead to non-radiative recombination caused by energy level mismatches. The accumulation of ion defects at the interface contact reduces charge extraction and indirectly affects the photocurrent and fill factor. This also limits the attainment of maximum open-circuit voltage and decreases stability on the surface of perovskite thin films. Therefore, in this study, we employ organic amine compounds to passivate ion defects on the surface of CsFAPbIxBr3-x perovskite thin films. We found that the sulfur atoms in the negatively charged diethyl dithiocarbamate (DADA) can interact with under-coordinated lead ions through Lewis acid-base interactions, effectively passivating iodine vacancies and to improve the efficiency of components in the atmosphere, simple additives can be used to help create more stable perovskite solar cells.
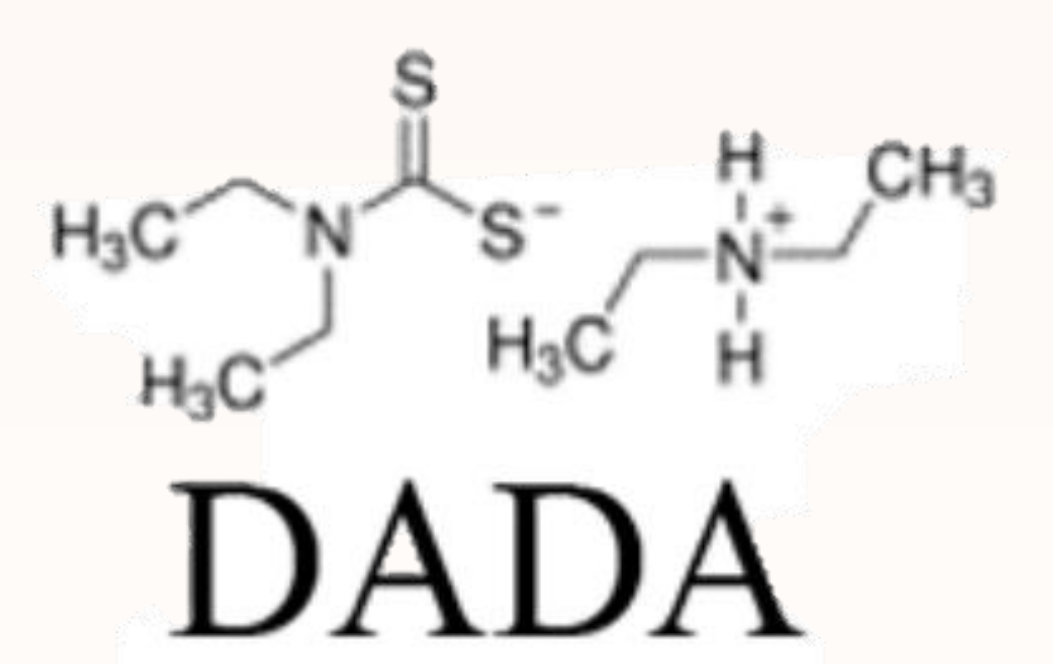
Figure 1. Molecular structure of diethylamine diethyldithiocarbamate (DADA)
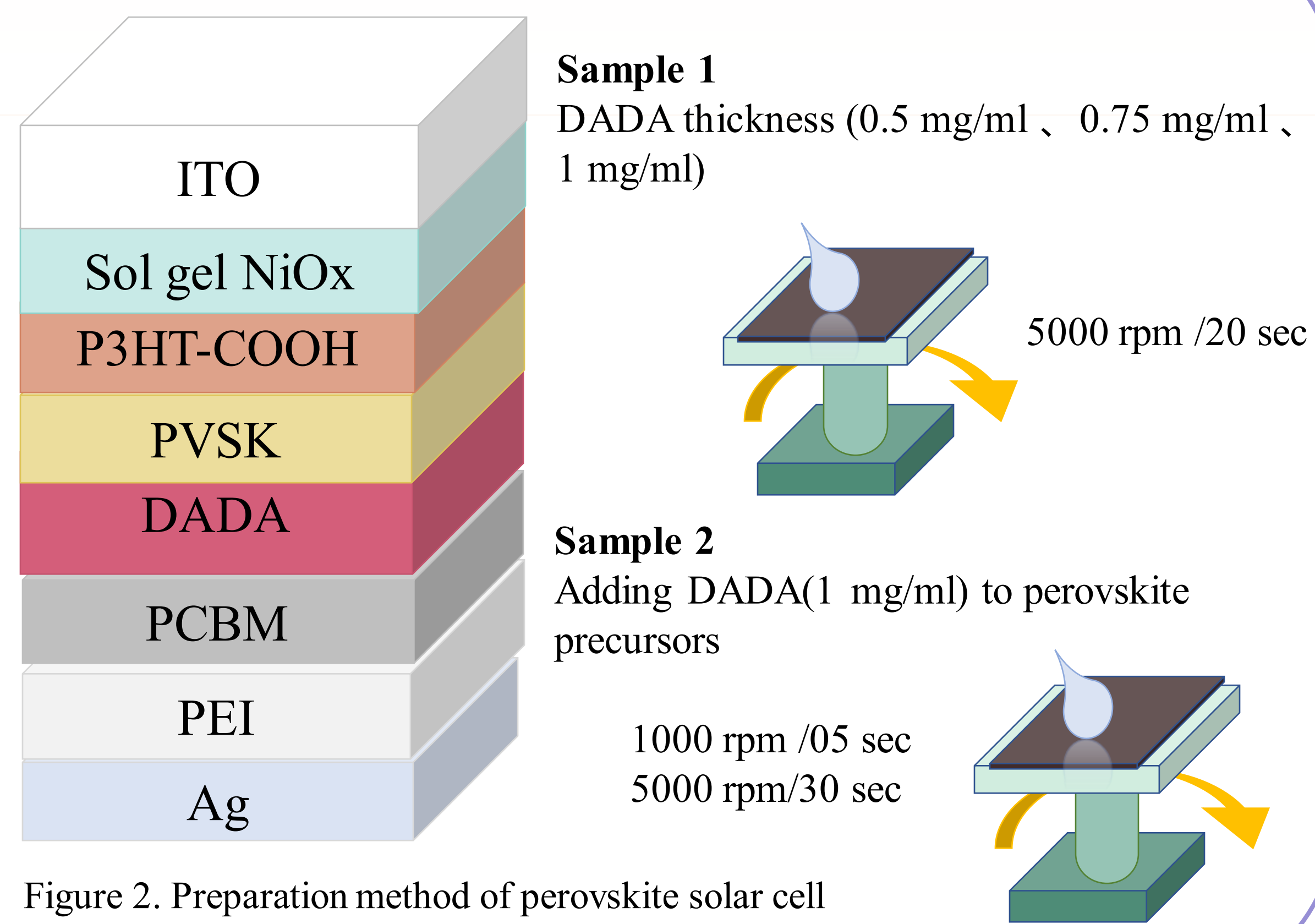
Experimental Method

ITO
Sol gel NiOx
P3HT-COOH
PVSK
DADA
PCBM
PEI
Ag

Sample 1
DADA thickness (0.5 mg/ml 、 0.75 mg/ml 、 1 mg/ml)

5000 rpm /20 sec

Sample 2
Adding DADA(1 mg/ml) to perovskite precursors

1000 rpm /05 sec
5000 rpm/30 sec

Figure 2. Preparation method of perovskite solar cell components in the glove box.

Device characteristics

Table 1. Component characteristics with different DADA concentrations.

Average value Sample	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
DADA(0.5 mg/ml)	1.01±0.03	15.26±0.08	64.68±2.22	10.02±0.52
DADA(0.75 mg/ml)	1.1±0.01	16.45±0.59	84.29±5.05	15.27±0.98
DADA(1 mg/ml)	1.1±0.01	17.11±0.27	82.1±9.6	15.5±1.99
DADA(1.5 mg/ml)	1.03±0.08	15.27±1.3	65.33±17.78	10.12±2.76

Table 2. The relationship between the efficiency of adding DADA elements to the precursor and time under atmospheric pressure.

Average value Sample	T : 25~28 ℃、 RH : below 20%			
	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
PVSK Day 0	1.09±0	15.48±0.06	84.16±0.59	14.25±0.15
PVSK Day 3	1.03±0.01	17.16±0.12	47.82±0.67	8.43±0.07
PVSK Day 7	0.93±0.08	6.62±0.88	17.48±2.7	1.05±0.14
PVSK+DADA Day 0	1.06±0.02	17.18±0.28	74.07±6.8	13.49±1.53
PVSK+DADA Day 7	1.06±0.01	16.42±0.31	63.83±0.65	11.04±0.26

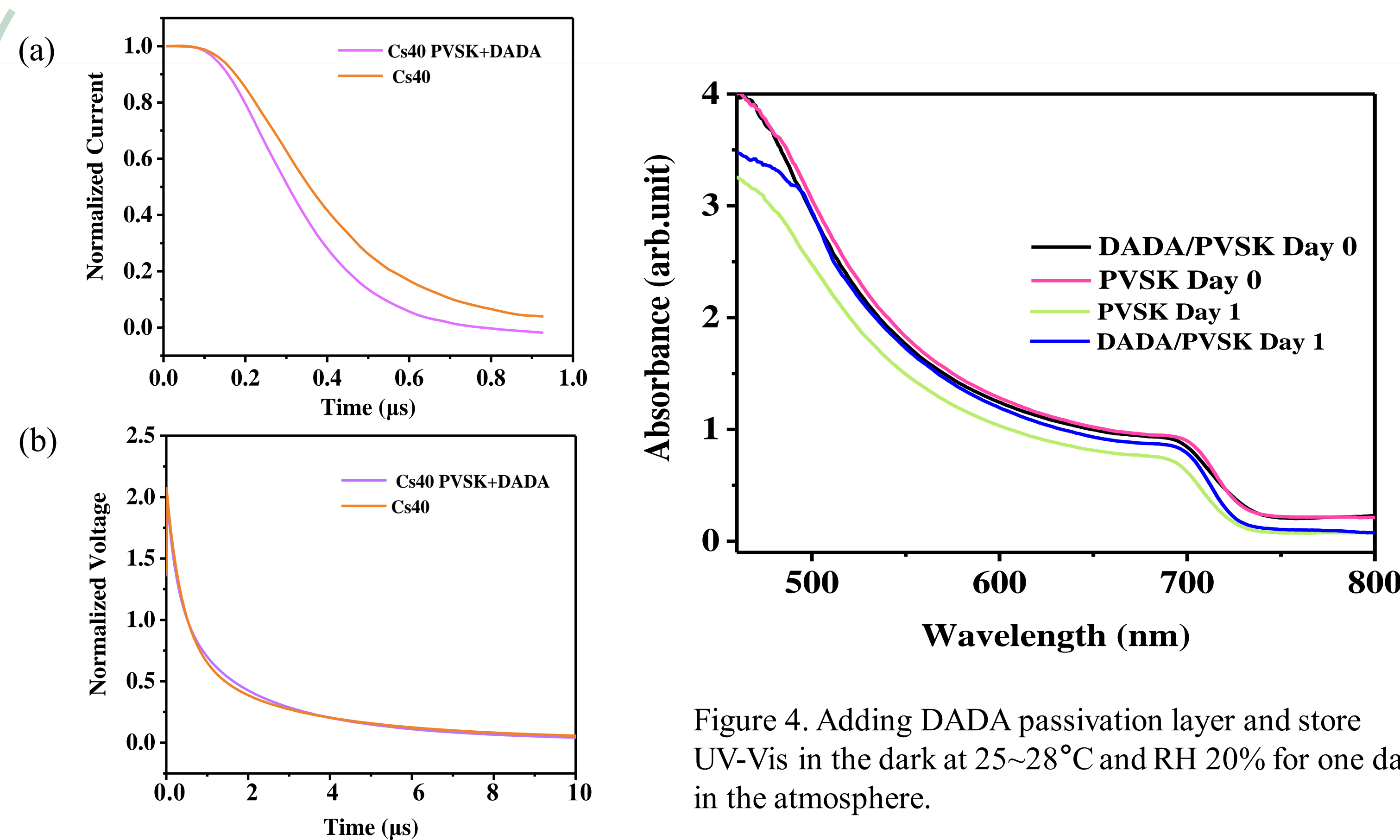## Optical properties and electrical analysis

Figure 3. Adding DADA (a) TPV and (b) TPC to the precursor.

Figure 4. Adding DADA passivation layer and store UV-Vis in the dark at 25~28°C and RH 20% for one day in the atmosphere.

Figure 5. The storage situation of components in the glove box; Sample 1 is a component with a DADA passivation layer added at 1 mg/ml, and Sample 2 does not have a DADA layer added.

Table 3. Relationship between component yield and time.

Aging condition	Sample	Initial PCE (%)	T80 (Day)	T50 (Day)
Glove box	1	14.95±0.91	7	
Glove box	2	15.34±0.54	4	

Surface topography
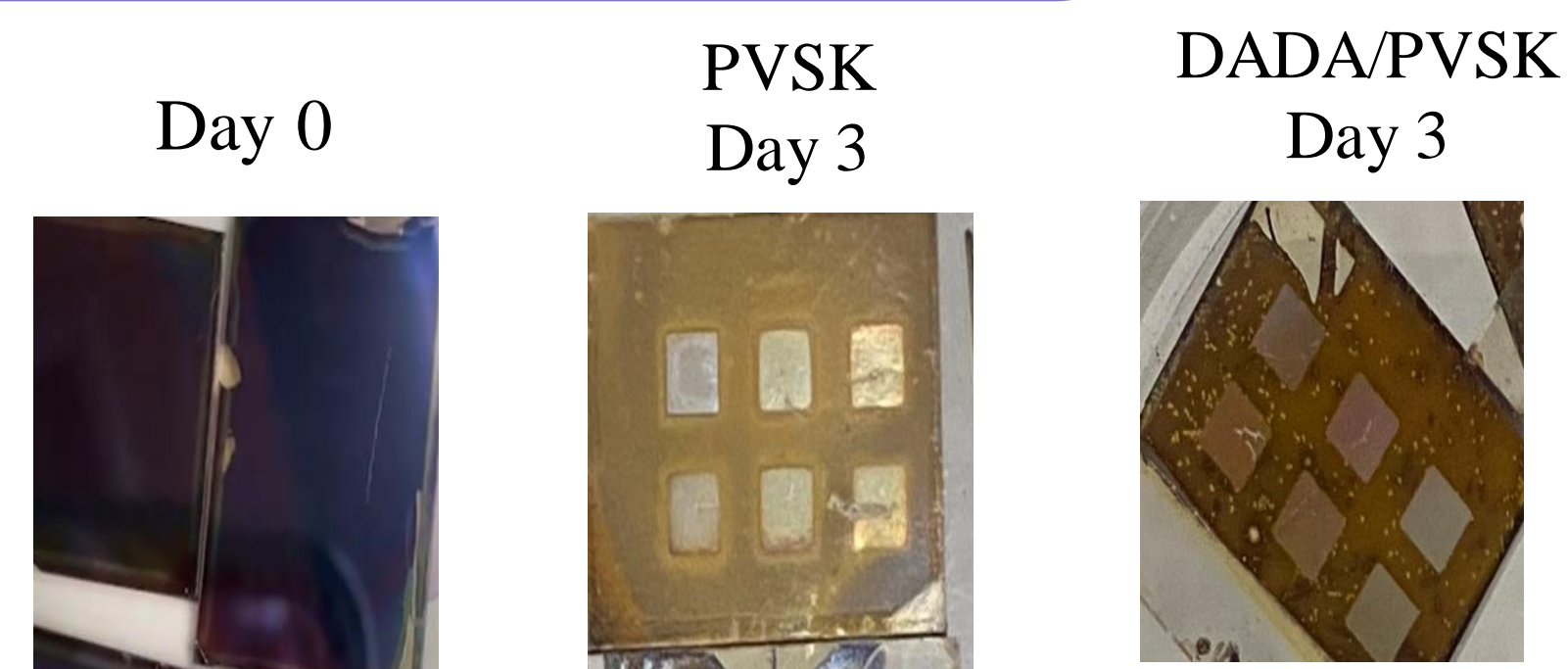

Day 0   PVSK Day 3   DADA/PVSK Day 3

Figure 6. The morphology of the component changes when it is placed in the atmosphere at 25 ~ 28°C and RH20% for three days.

Conclusions

- Adding DADA after the active layer or precursor of a perovskite solar cell can make the storage yield of the component 60% higher than that of the component without it when stored in the atmosphere at 25~28°C and RH20%; and adding a DADA passivation layer The components can also have better perovskite phase stability in the atmosphere, and better perovskite phase preservation on the third day.

- Through this test, it can be found that although adding a passivation layer, etc. can optimize the components, if the ambient temperature or humidity is raised to above 85°C and RH 85%, the components will degrade within 2 to 3 hours, and the stability still needs to be improved through packaging. It cannot be directly placed in a high temperature and high humidity environment through the above method; however, this research can still improve the stability of the component against high temperature and high humidity during packaging.

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