

Research on TiO₂ Nanocrystalline Solar Cell

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Abstract: This article researches the working principle of TiO₂ nanocrystalline solar cell, I-V curves and redox electrolytes. Moreover, it also provides reference to of TiO₂ nanocrystalline solar cell, especially to the further development of dye-sensitized solar cell.

1. Introduction

Fossil energy is the main energy source used by human beings at present. By the middle of the 21st century, fossil energy will be reduced to half of the energy that we use. Energy is one of the top 10 problems that mankind will face in the future. Humanity will mainly rely on nuclear and renewable energy. In the future, renewable energy will account for more than 1/3 of energy use [1-2]. People generally believe that: “solar energy inexhaustible”. Plants use photosynthesis to convert energy. Solar energy is a thousand times more energy than all other renewable energy sources. At present, human technology can realize the conversion of solar energy into heat energy. The application of photovoltaic effect greatly promotes the utilization of solar energy. Solar cells are easy to store and transport, making the use of solar energy more convenient. Solar cells mainly use photoelectric effect or photochemical effect to convert light energy directly into electricity. China's energy development plan calls for a solar cell capacity of 1.8GW by 2020. At present, most solar cells on the market are silicon-based solar cells, and crystalline silicon solar cells are the most common.

There are various ways to classify solar cells, which can be divided into silicon solar cells, polymer multi-layer modified electrode solar cells, multi-compound thin film solar cells and nanocrystalline solar cells according to the different materials used. Silicon solar cells obtain the most mature technology and dominate the market. Nano TiO₂ crystal chemical solar cells are mainly dye-sensitized solar cells (DSSC). The main advantages of fuel-sensitive solar cells are low cost and stable performance. If its photoelectric efficiency and stability can be improved by more than 10%, its production cost only accounts for 1/5 ~ 1/10 of the cost of silicon solar cells. And the life span can reach more than 20 years. Therefore, Nano TiO₂ crystal chemical solar cells are favored by solar cell researchers all over the world.

Table 1 Main Solar Cell Comparison

Technical route		Maximum conversion efficiency in the laboratory	Batch production efficiency	Component costs(US Dollar/W)	Merit and demerit
Silicon solar cell	Monocrystalline silicon cell	24.70%	17%	2.29	High silicon consumption and high cost
	Polysilicon cell	19.30%	14%	2.25	High silicon consumption and high cost
Diversified thin-film solar cells	Amorphous silicon thin-film cell	12.80%	6%-7%	1.0-1.5	Low silicon consumption, large investment and attenuation
Polymer multilayer modified electrode solar cell		40.70%	30%	3	High efficiency, high cost

2. Operating principle

Figure 1 shows the working principle of DSSC solar cell. The photocurrent generation process is as follows: Material (S) from ground state to excited state (S^*). At this time, electrons are injected into the conduction band of the semiconductor, and the oxidized dye is reduced by I^- ion, so that the dye cycle can be realized. Electrons in the conduction band (CB) are transferred to the back contact (BC) in the nanocrystalline network and flow into the external circuit. Electrons transferred in nanocrystalline films recombine with I_3^- ions in titanium dioxide film holes (rate constant is K_{et}). The diffusion of I_3^- ions to the opposite electrode (CE) causes electron circulation. If the dye excited state of the longer life, the more conducive to the injection of electrons. If the lifetime of the excited state is shorter, the excited state molecule may not be able to inject electrons into the conduction band of the semiconductor by non-radiation-attenuated transition to the ground state. ②, ④ are key to determine the efficiency of electron injection. The chance of charge recombination is related to the ratio of the electron injection rate constant (K_{inj}) to the inverse reaction rate constant (K_B) (generally larger than 3 orders of magnitude). The higher the ratio, the smaller the chance of charge recombination and the higher the efficiency of electron injection. As the dye can be recycled through the I^- ion reduction oxidation state of the dye, electrons are continuously injected into the titanium dioxide conduction band. The degree of electron return inhibition increases with the rate constant of I^- ion reduction oxidation dye. We can see it as I^- ions on electronic comes to intercept (interception). Due to the current loss in step 6, the higher the transmission speed of electrons in the nanocrystalline network (step ⑤) is. Moreover, the smaller the rate constant of the electron composite I_3^- ion (K_{et}), the greater the photo generated current. The resulting I_3^- ions are diffused to the opposite electrode (step 3) and the electrons become i^- ions (step 7), thus making the I^- ions form a current circulation.

These two functions are performed in dye-sensitized solar cells [5]. Firstly, the sensitizer completes the capture of light. After the light excitation, the dye molecule transitions from the ground state to the excited state (i.e. the charge separation state). If the two energy levels match and the excited state of the dye molecule is higher than the conduction band bottom of the semiconductor, the dye in the excited state will inject electrons into the conduction band of the semiconductor. The electron injected into the conduction band has the following characteristics: The transmission in the membrane is rapid, and it can immediately reach the back contact between the membrane and the conductive glass, thus entering into the external circuit. The main functions of semiconductors are load sensitizers, electron collection and conduction. According to theoretical analysis, the photo-voltage of the battery should be the difference between the quasi-fermi level of TiO_2 under illumination and the Nernstian potential of redox couple in electrolyte solution [3-6].

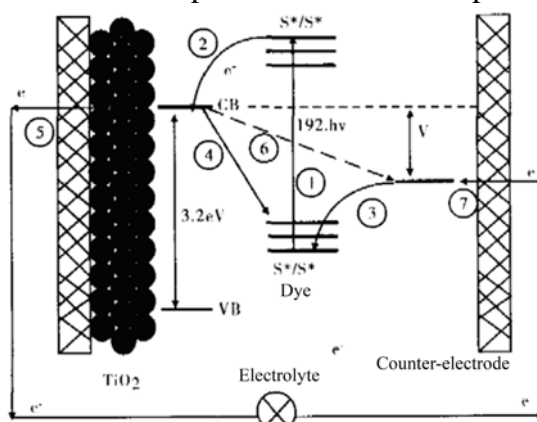


Figure 1. Working principle of DSSC solar cells

3. I -- V curve.

The photoelectric conversion ability of the electrode can be described by photocurrent working spectrum. The photoelectric conversion of dye-sensitized semiconductor electrodes at different

wavelengths can be analyzed from the photocurrent working spectrum. Firstly, the output photocurrent and photo-voltage of the battery are measured, and then the $I-V$ curve is made. Finally, the application value of dye-sensitized solar cells is analyzed.

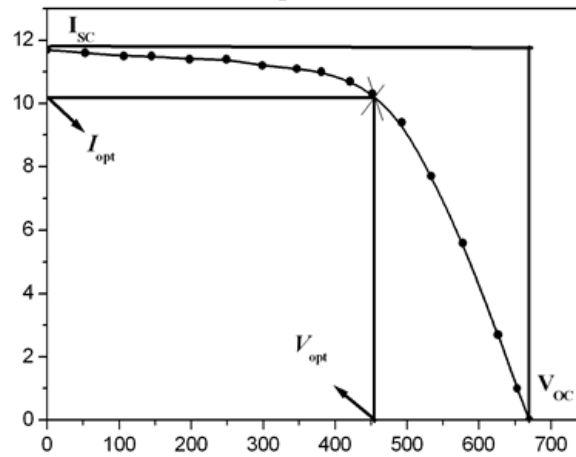


Figure 2. The $I-V$ curve of a typical solar cell

Figure 2 is the $I-V$ curve of a typical solar cell. Filling factor is the parameter that reflects the performance of solar cell (FF). The value is equal to the ratio of the product of the current (I_{opt}) and voltage (V_{opt}) and the product of the short-circuit photocurrent and the open-circuit photo-voltage when the battery has the maximum output power (P_{opt}).

$$FF = P_{opt} / (I_{sc} \times V_{oc}) = (I_{opt} \times V_{opt}) / (I_{sc} \times V_{oc}) \quad (1)$$

Another parameter that characterizes the performance of solar cells is the conversion efficiency of light energy to electricity. The value is the ratio of the maximum output power of the battery to the input light power (P_{in}), sometimes called energy conversion efficiency.

$$\eta = P_{opt} / P_{in} = (FF \times I_{sc} \times V_{oc}) / P_{in} \quad (2)$$

Let's illustrate figure 2 below. The intercept of the $I-V$ curve represents the short circuit photocurrent. The intercept of the $I-V$ curve on the x axis represents the open circuit optical voltage. The voltage is zero in short circuit and the current is zero in open circuit. The turning point of the curve (x) corresponds to the current and voltage of the maximum output power. The rectangular area corresponding to this point is the maximum output power. In theory, the maximum power a battery can generate should be the rectangular area of the point at which there is a short-circuit photocurrent and an open-circuit photovoltage (there is no such point). The ratio of the actual maximum power (the area corresponding to the inflection point) to the theoretical power (the maximum area) is called the filling factor. The filling factor is an important parameter for the output performance of reactive cells. The most important parameters of the battery are short-circuit photocurrent and open-circuit photovoltage. The basic condition of improving energy conversion efficiency is to increase the short circuit photocurrent and open circuit photovoltage. If the short-circuit photocurrent and the open-circuit photovoltage have the same two cells, the filling factor is the factor affecting their efficiency. The larger the filling factor, the higher the energy conversion efficiency. Generally, the total energy conversion efficiency represents the energy conversion efficiency under white light, while the energy conversion efficiency under monochromatic light is distinguished by it.

4. Redox electrolyte

The dye is oxidized by injecting electrons into the conduction band of the titanium dioxide semiconductor. Redox electrolytes must be used to reduce the oxidized dyes in order to continuously recycle the photoelectric conversion energy. I_3/I^- redox couple is the most common REDOX electrolyte used in dye-sensitized solar cells. Increasing I^- ion concentration can accelerate

the reduction of oxidized dyes and reduce the charge recombination on the electrode surface. Lower I_3^- ion concentration and increase open circuit photo-voltage. This can be explained by the following formula (3) for calculating the open-circuit optical voltage.

$$V_{oc} = \left(\frac{kT}{e} \right) \ln \left(\frac{I_{inj}}{n_{cb} k_{et} [I_3^-]} \right) \quad (3)$$

I_{inj} is the injected electron flow, n_{cb} is the electron concentration in the conduction band, k_{et} is the rate constant of the reaction between injected electron and I_3^- ion, and $[I_3^-]$ is the equilibrium concentration of I_3^- on the surface of nanocrystalline film.

By analyzing the variation rule of I_3^- ion concentration in dye-sensitized solar cells, we obtained an appropriate I_3^- ion concentration for different dye systems. In aqueous solution, the flat band potential of semiconductor is less affected by metal ions and more affected by pH value of solution. In aprotic solvent, metal ions have great influence on the flat band potential of semiconductor. The value of the flat band potential mainly depends on metal ions, and the positive trend of the flat band potential increases with the increase of the concentration of metal ions. But the flat band potential is not affected by anions. The adsorption of metal ions to the surface of titanium dioxide nanocrystals not only changes the conduction band level, but also inhibits the reverse electron transfer and charge compound reaction. Meanwhile, the reduction reaction of I^- ions to oxidized dyes is accelerated, which is beneficial to the generation of photocurrent. The conduction band energy level is different with the different cation adsorbed on the surface of titanium dioxide nanocrystalline. This also explains the change of photoelectric conversion efficiency.

I_3^-/I^- is the main redox couple in liquid electrolyte. The electrode potential of I_3^-/I^- redox couple matches not only the energy level of nanometer semiconductor electrode, but also the energy level of reductive and oxidized dyes. Because I^- reduces oxidized dyes, the main properties of solar cells are restricted by the reductive activity of I^- and the cation in iodide.

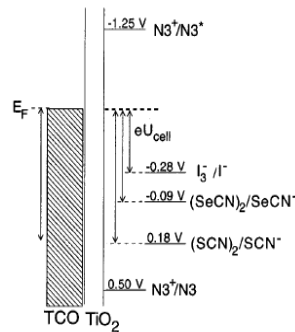


Figure 3. Comparison of energy levels

In conclusion, the stability and production cost of dye-sensitized nanocrystalline solar cells should be considered. The choice of solid or quasi-solid electrolyte has a broader application prospect than that of liquid electrolyte.

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