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A Study of perovskite solar cell with Fe^{3+}/Ga^{3+} doped TiO_2 layer

Seong Gwan Shin[1], Haram Lee[1] and Hyung Wook Choi[1]

[1] Univ. of Gachon
SeongnamDaero, Sujeong-Gu
Seongnam-Si, Gyeonggi-Do, 13120, Republic of Korea
Phone: +82-31-750-6024 E-mail: chw@gachon.ac.kr

Abstract

Recently, organic-inorganic lead halide perovskite solar cells (PSCs) have emerged as an extremely attractive photovoltaic device. Perovskite has a structure of a large number of solar cells, which is very promising for the rapid commercialization of large-scale, low-cost solar cells. PSCs have many advantages as it uses simple processing techniques and inexpensive raw materials. The conduction band of TiO_2 used in many PSCs coincides well with the conduction band of the perovskite active layer. In addition, TiO_2 has excellent stability and conductivity and can be obtained by various deposition methods at a low cost. However, TiO_2 traps electrons in oxygen vacancies and Ti lattice sites, which leads to recombination, which in turn reduces the efficiency of the device. In this study, we investigated the effects of Fe^{3+}, Ga^{3+} ions on the efficiencies of PSCs by doping them in a compact and mesoporous layer of TiO_2. Fe^{3+}, Ga^{3+} with an atomic radius similar to that of Ti^{4+} can replace Ti cations, and Fe^{3+}, Ga^{3+} doped TiO_2 is considered to be a better candidate for photoelectric performance of PSCs.

1. Introduction

During the last three decades, the development of renewable energy technologies has received substantial attention to overcome the effects of energy crisis, environmental pollution, and global warming. Among the various renewable and sustainable energy resources, solar power is the most remarkable, because of its abundance, global availability, and cleanliness. [1] Recently, organic-inorganic lead halide perovskite solar cells (PSCs) have emerged as an extremely attractive photovoltaic device. [2-5] Perovskite has a structure of a large number of solar cells, which is very promising for the rapid commercialization of large-scale, low-cost solar cells. PSCs have many advantages as it uses simple processing techniques and inexpensive raw materials. Perovskite materials have the general formula of ABX, where A is generally methyl ammonium (CH_3NH^{3+} or MA), B is a metal ion, such as Pb or Sn, and X represents a halogen ion, such as I, Cl, or Br. A distinct advantage of lead-based perovskites (i.e., $MAPbX_3$) is that their band gap can be easily tuned from 1.2 to 2.3 eV by varying the composition of cations and anions. [6-7] The conduction band of TiO_2 used in many PSCs coincides well with the conduction band of the perovskite active layer. In addition, TiO_2 has excellent stability and conductivity and can be obtained by various deposition methods at a low cost. In this regard, in many PSCs, TiO_2 is widely used as the ETL owing to its excellent electronic properties.[8-11] However, TiO_2 traps electrons in oxygen vacancies and Ti lattice sites, which leads to recombination, which in turn reduces the efficiency of the device. Therefore, the generation of oxygen vacancies and reduction in the number of defects of TiO_2 facilitate the development of stable PSCs. Many studies have shown that the efficiency can be effectively improved by reducing the recombination of TiO_2 by doping appropriate metal ions.

In this study, we investigated the effects of Fe^{3+}, Ga^{3+} ions on the efficiencies of PSCs by doping them in a compact and mesoporous layer of TiO_2. Fe^{3+}, Ga^{3+} was dissolved in ethanol and mixed with a TiO_2 solution in various ratios. The metal ion can effectively enhance the electron transfer of TiO_2. Fe^{3+} with an atomic radius similar to that of Ti^{4+} can replace Ti cations, and Fe^{3+}, Ga^{3+} doped TiO_2 is considered to be a better candidate for photoelectric performance of PSCs. Upon the doping with Fe^{3+}, the conductivity increased and the recombination decreased, which increased the efficiency of the PSC.

2. Results & discussion

The XRD measurement is performed to reveal the lattice structure. As shown in Figure 1 (a), the Ga^{3+}, Fe^{3+}-doped TiO_2 layer consists of the anatase phase, as the Ga^{3+}, Fe^{3+} ion radius is very similar to that of Ti^{4+} and thus the Fe^{3+} dopant cannot change the lattice of TiO_2.

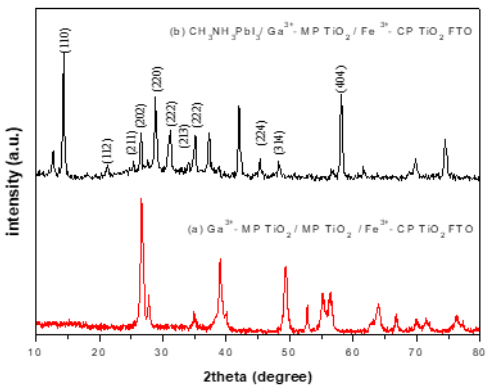

Fig. 1 XRD patterns of $MAPbI_3$, Fe^{3+}, Ga^{3+} - TiO_2.

Figure 1 (b) shows the XRD pattern of $TiO_2/CH_3NH_3PbI_3$ with peaks at 13.8, 19.7, 23.1, 24.2, 28.1, 31.5, 40.3, and 42.8° attributed to the (110), (112), (211), (222), (224), and (314) lattice planes, respectively.

Figure 2 (a) is a mesoporous TiO_2 layer made of diluted 18NR-T. Figure 2 (b) is a cross-sectional view of a mp-TiO_2/

Ga-doped mp-TiO_2 layer prepared by spin-coating a mesoporous 18NR-T. Figure 2 (b) is a cross-sectional view of a mp-TiO_2/Ga-doped mp-TiO_2 layer prepared by spin-coating a mesoporous TiO_2 layer prepared by adding gallium nitrate to a solution of the same concentration. figure 2(C) is a cross-sectional view of the PSC produced, and CP-TiO_2 layer was prepared by mixing iron nitrate and TiO_2 sol. The Fe^{3+} doped TiO_2 / mesoporous TiO_2 / Ga^{3+} doped TiO_2 / perovskite / HTL / electrode structures were fabricated.

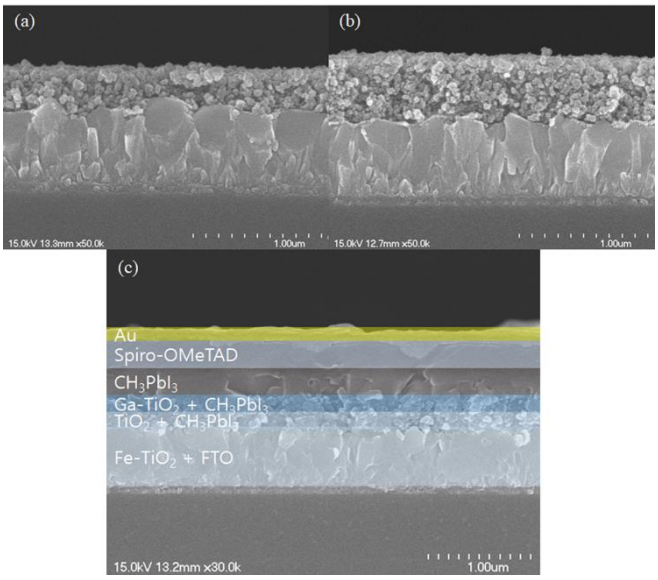

Fig. 2 Scanning Electron Microscope images of (a) mesoporous TiO_2 layer, (b) Gallium doped mesoporous TiO_2 layer on mesoporous TiO_2 layer and (c) Fabricated perovskite solar cell.

Figure 3 is a graph of the absorbance of the TiO_2 layer. It can be seen that the bandgap changes when iron is doped and when gallium is doped, which suggests that a valence band can be distributed between the FTO and the perovskite layer.

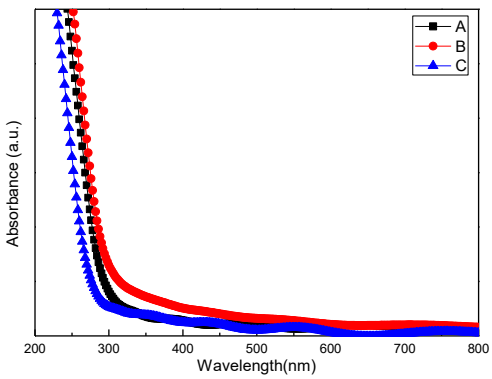

Fig. 3 The absorbance graph of (a) mesoporous TiO_2 layer, (b) Fe doped TiO_2 layer and (c) Ga doped TiO_2 layer.

The J-V curve in Figure 4 shows that the PSCs photovoltaic properties are improved. The corresponding photovoltaic properties are summarized in Table I. Oxygen vacancies or Ti lattice sites are converted to Ti^{3+} by stoichiometric defects in the TiO_2 lattice. Therefore, the Ti^{3+} lattice defects can induce low energy levels and the conduction band can trap electrons and reduce the electron transport efficiency, leading to recombination. The increase in open-circuit voltage (V_{oc}) is worth discussing. When TiO_2 is doped with metal cations, the TiO_2 energy level is changed and the V_{oc} value is increased.

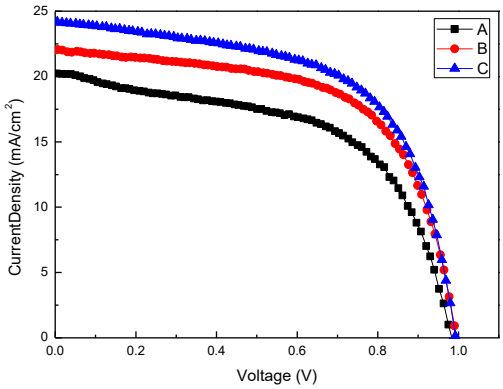

Fig. 4 J–V curves of the PSCs of (a) CP TiO_2/MP TiO_2, (b) Fe^{3+}-CP TiO_2/MP TiO_2, (c) Fe^{3+}-CP TiO_2/Ga^{3+}-MP TiO_2.

Table I Current density-voltage characteristics of best performing perovskite solar cell

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	η (%)
(a)	0.978	24.25	48.37	11.47
(b)	1.010	23.18	60.19	13.84
(c)	0.993	24.16	59.96	14.39

3. Conclusions

We fabricated PSCs based on $MAPbI_3$ using Fe^{3+} and Ga^{3+}. The TiO_2 layer doped with Fe^{3+} and Ga^{3+} has a uniform surface, and electron recombination is reduced to improve electrical conductivity. The PSC exhibited a short-circuit current density (J_{sc}) of 24.16 mA/cm^2, V_{oc} of 0.993 V, FF of 59.96%, and efficiency (η) of 14.39%. Therefore, the use of the Fe^{3+}, Ga^{3+}-doped TiO_2 layer is a promising approach for fabrication of high-performance PSCs.

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