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Non-pn-junction-based Solar Cells: Charge Carrier Separation in Solar Cells with Bound Surface Charges

Fude Liu,1 Wentao Wang,1 Chor Man Lau,1 Lei Wang,1 Guandong Yang,1 Dawei Zheng,1 Zhigang Li2

1Department of Mechanical Engineering, The University of Hong Kong, Hong Kong, China
2Department of Mechanical Engineering, The Hong Kong University of Science and Technology, Hong Kong, China

Abstract — Traditional junction-based solar cells have limitations on picking the right materials and processing steps to form a working junction due to, for example, lattice mismatch, doping, and band alignment. In this work, we then demonstrated a new approach to realize the charge carrier separation in solar cells with the bound surface charges on ferroelectric. The appearance of bound surface charges leads to an induced voltage $V$ between the two surfaces of the ferroelectric. The induced voltage $V$ is then applied on the semiconductor as an external electric field to enhance the charge separation in the semiconductor. Detailed theoretical calculations and experimental results verify the feasibility of the new concept, although the device performance is still poor at the moment. We are therefore confident that our new concept cell is promising because of its many advantages over traditional junction-based solar cells such as more options in choosing semiconductors for solar cells, more flexibility in device design, good potential in achieving high performance, and simple processing steps.

Index Terms — photovoltaics, ferroelectric, bound surface charge, silicon.

I. INTRODUCTION

Solar photovoltaics (PV) is expected to play an important role in our energy future [1-4]. However, the market share of solar electricity in our energy pattern is still small mainly due to its high cost compared to traditional fossil fuel energy. Although many kinds of solar cells have been developed in the past several decades, we find that almost all the cells are essentially junction-based [5-11]. However, the junction-based structure is just one way to realize the functions of solar cells. In addition, this kind of structure limits our choices on picking the right materials and processing steps to form a working junction. Therefore, it is worth exploring other possibilities in order to realize the ultimate goal of photovoltaics, i.e., reducing cost and increasing scalability [12-16].

We present herein a new type of photovoltaic device — field-effect solar cells with ferroelectrics. The device takes advantages of both ferroelectric and semiconductor materials. Like traditional solar cells, the new device still uses semiconductor materials as the light-absorbing layer, because of their suitable energy bandgaps and excellent carrier transport. In addition, ferroelectric materials are introduced to provide an external electric field on the semiconductor layer to enhance the charge carrier separation therein, because bound surface charges appear on the ferroelectric surface due to polarization. Unlike the case in traditional ferroelectric cells though, the ferroelectric layer in our devices is not used as the light absorber because of its large bandgap and poor sunlight absorption. Our new devices therefore can overcome the above-mentioned problems displayed by conventional photovoltaic cells, and they are thus promising in providing better energy conversion efficiency as far as carrier generation, separation and transport are concerned. The new concept provides more flexibility in producing solar cells with broad applications and is promising in achieving high-efficiency solar cells at low cost.

II. EXPERIMENTAL

We prepared several solar cells (see Fig. 1). The semiconductor is p-type single-crystalline silicon wafer with thickness of 170 µm. The ferroelectric is 500 nm-thick BaTiO₃ spin coated on the wafer with the sol-gel method. The BaTiO₃ film was annealed at > 700 °C for crystallization. All contacts are made of the same metal Al (120 nm thick) to rule out the possible effect on the device performance caused by the work function differences of contacts. The distance between the anode and cathode is 1.5 mm and the width of the metal line 0.5 mm. The backside of the whole device is covered by epoxy for insulating. The ferroelectric was poled by following the standard procedure [17]. The effective area of the device was estimated to be ~78 mm².
III. RESULTS AND DISCUSSION

We measured the $I$-$V$ curves of the device with a standard solar simulator. The test results are shown in Fig. 2. Under dark condition and before poling, we see that the $I$-$V$ curve is in general Ohmic (the upper figure of Fig 6b). However, after poling, the curve shows rectifying properties as in a pn-junction diode. Under illumination condition, the pre-poling $I$-$V$ curve shifts downward only slightly while the post-poling curve shifts much more (the lower figure of Fig 6b). The important values for the poled cell are as follows: Open-circuit voltage ($V_{oc}$) = 56 mV, short-circuit current ($I_{sc}$) = 1.21×10^{-2} mA, and fill factor (FF) = 24 %. We repeated the experiment with several samples (even with different metal contacts) and the results turned out to be consistent and repeatable. Therefore, we conclude that our proposed solar cell works.

We study theoretically the feasibility of the new solar cell. We assume that the ferroelectric is blocking and do not allow electrons or holes to be injected/exchanged between the electrodes (or semiconductor) and the ferroelectric. First, we calculate the maxim electrostatic potential $V$ due to the ferroelectric polarization. As shown in Fig. 1, the induced polarization $P$ leads to induced bound surface charges given by $Q_P = A P$, where $A$ is the electrode area. The ferroelectric is assumed to be uniformly polarized in the direction perpendicular to the plane. Appearance of surface charges leads to a voltage (potential) difference $V$ between the two surfaces of the dielectric. If $C$ is the capacitance, then the induced voltage $V$ is,

$$V = \frac{Q_P}{C} = \frac{A P}{\varepsilon_0 \varepsilon_r A} = \frac{d P}{\varepsilon_0 \varepsilon_r}$$ \hspace{1cm} (1)
where \( d \) is the separation of the metal electrodes (plates), \( \varepsilon_0 \) the vacuum permittivity (= \( 8.85 \times 10^{-12} \) F/m), and \( \varepsilon_r \) the dielectric constant. We can get \( V = 3.9 \) V when \( d = 100 \) nm, \( P = 0.10 \) C/m\(^2\), and \( \varepsilon_r = 290 \) [18, 19]. These are the typical values for ferroelectric films. Alternatively, we can get the same result with Gauss's law [20]. The induced voltage \( V \) is adjustable, for example, by changing the thickness \( d \) of the ferroelectric. In comparison, in a typical Si pn junction the fixed ion charge density is \( \approx 10^{-4} \) C/m\(^2\), the potential change across the depletion region \( \approx 0.85 \) V, and the maximum value of the electric field at the depletion region \( \approx 10^4 \) V/cm [21]. Therefore, we have corresponding parameters to play around in our new solar cell.

IV. CONCLUSIONS

In summary, we have demonstrated a new type of photovoltaic cells that realize the charge carrier separation in the semiconductor with the bound surface charges of the ferroelectric. The feasibility of the new cells was verified both experimentally and theoretically in detail. The photovoltaic effect was experimentally observed for the cells after forward polarization only. In addition, it was shown in principle that suitable induced electric fields could be conveniently attained for charge separation in the new cells. In general, the new cells work in a similar fashion as traditional PN junction based counterparts. However, because of the unique physical separation between free charge carriers and fixed charge carriers in the new cells, we can go beyond traditional junction-based structures and have more freedom in material selection, device design and fabrication in photovoltaics. We therefore believe that the new concept is promising in enabling us to prepare novel solar cells and other solid-state devices.

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