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High-performance Piezo-phototronic Solar Cell Based on Two-dimensional Materials

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Abstract

Pieoztronic and piezo-phototronic are two emerging fields of flexible electronics and nanoelectronics using by piezoelectric semiconductor materials, such as ZnO, GaN, InN and CdS. Recent experiments shown piezoelectric and semiconductor properties of monolayer MoS$_2$, which have been applied as nanogenerator and piezotronic transistor. Two-dimensional piezoelectric semiconductor can be utilized for high-performance photovoltaic devices. In this paper, a two-dimensional material piezo-phototronic solar cell is studied theoretically based on a monolayer MoS$_2$ metal-semiconductor contact. The current-voltage characteristics, open circuit voltage, maximum output power, fill factor and power conversion efficiency have been studied for the piezo-phototronic solar cell. The modulation level of piezo-phototronic effect is presented to evaluate the performance under applied strain. The piezo-phototronic effect can increase the open circuit voltage 5.8% at strain of 1%. This principle can be a new way to develop high-performance two-dimensional solar cells.
Monolayer MoS$_2$ shows piezoelectric and semiconductor properties in recent experiments, which have been used for nanogenertor and piezotronic transistor. Two-dimensional piezoelectric semiconductor can be applied for piezo-phototronic solar cell. The modulation by piezo-phototronic effect can enhance the performance of monolayer MoS$_2$ solar cells.

**Keywords**

Piezotronic, Piezo-phototronic, solar cells; two-dimension material; MoS$_2$

1. **Introduction**

Piezoelectric semiconductor nanomaterials have been paid more and more attention over the past ten years, such as ZnO, GaN, InN and CdS. The new emerging fields of piezoelectronics and piezo-phototronics are established based on coupling of piezoelectric and semiconductor properties [1]. Since the invention of nanogenertors in 2006 [2-4], nanostructure piezoelectric semiconductors have been applied to multifunctional electromechanical devices, such as piezotronic field effect transistor [5], strain sensor [6], piezo-phototronic photocell [7], and LED [8]. Furthermore, integrated
chips have been developed by nanowires array, such as taxel-addressable matrices [9] and photon-strain sensor arrays [10].

Recent experiments have revealed the coupling between piezoelectric and semiconductor properties in the single-atomic-layer MoS$_2$ [11], which promote the applications in powering nanodevices, energy harvesting and tunable electronics. Due to its excellent electronic, optical, catalytic and mechanical properties [12], monolayer MoS$_2$ can be fabricated as transistors [13, 14], photodetectors [15], and integrated circuits [16].

The principle of solar cell applies the built-in electric field to separate electron-hole pairs induced by incident photons in the p-n junction or metal-semiconductor contact. For piezo-phototronic solar cell (PSC), piezoelectric field can effectively assist the separation of photon-generated carriers [17, 18]. It should also be noted that piezo-phototronic effect can also improve the performance of two-dimensional material photodetector. High-performance, flexible and low-cost solar cell is research focus for large-area application, for example, building-integrated photovoltaic system [19]. Monolayer MoS$_2$ single junction device can be a good candidate for design of high-efficiency flexible solar cell, especially piezo-phototronic effect enhancing solar cell. There are several novel characteristics of monolayer MoS$_2$. First, incident sunlight can be absorbed up to 5% by monolayer MoS$_2$ within 1 nm, which is higher absorption about 10 times than GaAs and Si at same thickness [20]. Second, monolayer MoS$_2$ can be applied 11% in-plane strain [21]. Furthermore, monolayer MoS2 and other two-dimensional materials, such as WSe$_2$ and MoSe$_2$ can be fabricated as stacked multilayers solar cells [21]. This structure offers a low-cost way comparing with multi-junction high-efficiency solar cell.

In this manuscript, a two-dimensional material piezo-phototronic solar cell presents based on piezo-phototronics effect in monolayer MoS$_2$ materials [22, 23]. The schematic of the design is illustrated in Fig.1. The basic structure is a monolayer MoS$_2$ between two metal electrodes on the substrate. The left side of unstrained device is metal-semiconductor contact and right side is Ohmic contact, as shown in Fig. 1(a). For two-dimensional semiconductor materials, the metal-semiconductor-metal structure is commonly used in experiments. Because two back-to- back Schottky diode have opposite output voltage, the one side of 2D MSM device is used as solar cell and other side is electrode, that is to say, Ohmic contact. The device structure can also be p-n junction by using p-type and n-type 2D piezoelectric semiconductor materials. The piezoelectric polarization
charges are induced at the contact of the piezo-phototronic solar cell under tensile and compressive
strain. Piezoelectric field is able to increase or decrease the Schottky barrier at the contact as shown in
Fig. 1(b) and Fig. 1(c), respectively. Piezoelectric field can enhance built-in potential, as well as
assist to separate electron-hole pairs in metal-semiconductor contact. The parameters of
piezo-phototronic solar cell are studied, such as current-voltage characteristics, open circuit voltage,
maximum output power, fill factor, and power conversion efficiency. The scale ratio to evaluate the
piezophototronic modulation on output characteristics has been studied for PSCs, and the open circuit
voltage of monolayer MoS$_2$ PSC increases 5.8% with strain of 1%. This principle may provide a
feasible design to fabricate high-efficiency and low-cost photovoltaic devices.

2. Piezo-phototronic modulation on two-dimensional materials solar cells

Semiconductor physics and piezoelectric theory are used to describe the properties of
piezo-phototronic solar cell [17]. Piezoelectric charge induced by external applied strain can increase
open circuit voltage of the solar cell, and thereby improve the performance. According to the
piezo-phototronic theory, the total current density of 2D material solar cell is given by [17]:

$$ J = J_{MS} \exp \left( \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon kT} \right) \exp \left( \frac{qV}{kT} \right) - 1 - J_{solar} $$

(1)

where $J_{MS}$ is the saturation current density of metal-semiconductor, $\rho_{piezo}$ is the density of the
piezoelectric charges, $W_{piezo}$ is the width of the charges distribution, $k$ is the Boltzmann constant, the
temperature $T$ is 300K, $\varepsilon$ is the relative dielectric constant, $V$ is applied voltage and $J_{solar}$ is the
short circuit current density.

The density of the piezoelectric charges of 2D MoS$_2$ $\rho_{piezo}$ can be obtained as [22]:

$$ q\rho_{piezo} W_{piezo} = -e_{11}s_{11} $$

(2)

where $e_{11}$ is piezoelectric constant, and $s_{11}$ is applied strain.

The open circuit voltage is given by:

$$ V_{oc} = \frac{kT}{q} \left\{ \ln \left( \frac{J_{solar}}{J_{p0}} \right) + \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon kT} \right\} $$

(3)

The ratio $\gamma$ can describe the modulation for open circuit voltage of piezo-phototronic solar cell
by piezoelectric charges:

\[
\gamma = \frac{q^2 \rho \text{piezo} W^2 \text{piezo}}{2 \varepsilon k T \ln \left( \frac{J_{\text{solar}}}{J_{\text{MS}}} \right)}
\]  

(4)

This ratio \( \gamma \) can describe the piezo-phototronic modulation on output characteristics of piezo-phototronic solar cell.

Further, the output power can be obtained as:

\[
P(V) = V \times J(V) = V \times J_{\text{MS}} \exp \left( - \frac{q^2 \rho \text{piezo} W^2 \text{piezo}}{2 \varepsilon k T} \left[ \exp \left( \frac{qV}{k T} \right) - 1 \right] - J_{\text{solar}} \right)
\]  

(5)

The voltage at the maximum output power \( V_m \) can be solved by the following equation:

\[
V_m + \frac{k T}{q} \ln \left( \frac{qV_m}{k T} + 1 \right) = \frac{k T}{q} \ln \left( \frac{J_{\text{solar}}}{J_{\text{MS}}} \right) + \frac{q^2 \rho \text{piezo} W^2 \text{piezo}}{2 \varepsilon k T}
\]  

(6)

Thus, \( V_m \) changes with piezoelectric charges under applied strain. The current density at the maximum output power \( J_m \) and the maximum output power \( P_m \) can be calculated, respectively:

\[
J_m = J_{\text{MS}} \exp \left( - \frac{q^2 \rho \text{piezo} W^2 \text{piezo}}{2 \varepsilon k T} \left[ \exp \left( \frac{qV_m}{k T} \right) - 1 \right] - J_{\text{solar}} \right)
\]  

(7)

\[
P_m = V_m J_m
\]  

(8)

The fill factor, which is defined as the ratio of the maximum output power to the product of short circuit current and open circuit voltage, can be expressed as:

\[
FF = \frac{P_m}{J_{\text{solar}} V_{oc}} = \frac{J_m V_m}{J_{\text{solar}} V_{oc}}
\]  

(9)

The power conversion efficiency (PCE) is extracted from the J-V curve. PCE is the general efficiency of the solar cell, which is defined as the ratio of generated electricity to incoming light energy:

\[
PCE = \frac{J_{\text{solar}} V_{oc} FF}{P_{in}}
\]  

(10)

3. Results and discussion
The open circuit voltage, maximum output power, fill factor, and power conversion efficiency are calculated in the our calculation by using typical constants: The temperature is 300K, the relative dielectric constant of MoS$_2$ is 3.3 \cite{16}, the width of piezo-charges distribution $W_{\text{piezo}}$ is 0.25 nm \cite{17,22}, and the piezoelectric constant along a-axis for monolayer MoS$_2$ is 0.56 C/m$^2$ \cite{24}.

The model for calculations is shown in Fig.2 (a). A monolayer MoS$_2$ piezophototronic solar cell is based on the M-S contact at left side and Ohmic contact at right side. Fig.2 (b) presents the $J$ – $V$ characteristics of the 2D PSC with applied strain varying from -1% to 1%, at a fixed short circuit current density as 3.15 mA/cm$^2$ \cite{25}. The output power as a function of voltage at a fixed photocurrent density is shown in Fig.2 (c), indicating that current density increases with strain. The maximum power is obtained at $V_m$. Using by Eqn. (3) and Eqn. (8), the dependence of the open circuit voltage $V_{oc}$ and maximum output power $P_m$ on the applied strain are shown in the Fig.2 (d), respectively. The change of $V_{oc}$ and $P_m$ demonstrate the improvement on performance of 2D PSC by piezo-phototronic effect.

Fig.3 (a) shows the modulation ratio $\gamma$ for piezo-phototronic solar cell changes with $W_{\text{piezo}}$ while externally applied strain increases from -1% to 1%. While 2D material is stretched, the improvement on performance of 2D PSC will increase linearly. The width of piezo-charges distribution $W_{\text{piezo}}$ is a key parameter of piezotronic and piezo-phototronic junction or contact. Fig.3 (b) shows $\gamma$ as a function of strain when $J_{\text{solar}}$ is 3.15 mA/cm$^2$ \cite{25} and 22.36 mA/cm$^2$ \cite{26}. The modulation ratio $\gamma$ depends on the width of piezo-charge distribution $W_{\text{piezo}}$, as shown in Fig.3 (c). Due to piezo-phototronic effect, the modulation on output characteristics also is influenced by the width of piezo-charge distribution. The width of piezo-charge distribution is determined by not only different piezoelectric semiconductor, but also the metal materials of contact \cite{27,28}. The piezo-phototronic effect increases the open circuit voltage about 5.8% with strain of 1% while $W_{\text{piezo}}$ is 0.25 nm. For $W_{\text{piezo}}$ of 0.5 nm, the improvement on performance will reach up to 11.6% for this 2D PSC case. While strain of 2D material can be stretched to 11%, the ratio will reach even up to 10 times on the above case. This mechanism may provide a new way to develop high output performance.
two-dimensional solar cells.

Fig. 3 (d) shows the ratio \( \gamma \) as a function of strain for different 2D materials: MoS\(_2\), MoSe\(_2\), and WSe\(_2\). The piezoelectric constant is 0.56 C/m\(^2\) (MoS\(_2\)), 0.48 C/m\(^2\) (MoSe\(_2\)) and 0.27 C/m\(^2\) (WSe\(_2\)) [24], respectively. Therefore, the modulation ratio \( \gamma \) can be considered as a scale factor for piezo-phototronic solar cell. It’s obvious that the performance of piezo-phototronic solar cell can be tuned effectively by the applied strain in two-dimensional piezoelectric semiconductor materials. By solving the Eqn. (9) and Eqn. (10), two parameters to evaluate the performance of PSCs: FF and PCE are illustrated in Fig.4 (a) and Fig.4 (b), respectively, with the applied strain varying from -1.0% to 1.0%. The piezo-phototronic effect is able to improve fill factor and power conversion efficiency by increasing open circuit voltage, as a result, enhance the output performance of piezo-phototronic solar cell based on two-dimensional materials.

Piezoelectric properties have been discussed in other monolayer TMDs, such as MoSe\(_2\) and WSe\(_2\) [24]. The performance of piezoelectric solar cells fabricated by MoS\(_2\), WSe\(_2\)[29] and MoSe\(_2\)[30] presents in Table.1. It shows that the modulation ratio of MoS\(_2\) PSC is 2 and 4 times higher than MoSe\(_2\) and WSe\(_2\) PSCs. Table 2 presents the comparison between the recent experimental results based on piezoelectric semiconductor: MoS\(_2\)/InP [31], MoS\(_2\)/GaAs [32], MoS\(_2\)/Si and MoS\(_2\)/Graphene heterojunctions [25]. MoS\(_2\)/GaAs and MoS\(_2\)/InP have higher photocurrent density, which have the feasibility of applying piezo-phototronic effect to design the high performance ultra-thin solar cell.

4. Summary

In summary, we have presented the theoretical model of current-voltage characteristics of 2D piezoelectric solar cells. The open circuit voltage, maximum output power density, fill factor and power conversion efficiency are calculated for piezophototronic solar cells based on monolayer MoS\(_2\). Piezophototronic solar cells have superior improvement on performance applied by piezophototronic effect, especially in open circuit voltage. Furthermore, monolayer MoS\(_2\) shows potential for high performance piezophototronic solar cell comparing other two-dimensional materials. The theoretical results provide not only the physical picture for understanding the piezotronic and piezophototronic effect in two-dimensional solar cells but also the guidance for design of two-dimensional piezophototronic nanodevices.
Reference

Dongqi Zheng is a junior student in University of Electronic Science and Technology of China. He majors in electronic and information science and technology. His recent research interests are the theoretical calculation of piezotronics, and energy harvesting.

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Figure caption

Fig. 1. (a) Schematic and energy band diagram of a two dimensional piezophototronic solar cell fabricated using a monolayer MoS$_2$ metal-semiconductor contact at left side and Ohmic contact at right side. (b) Schematics and energy band diagram of the piezophototronic solar cell under compressive strain. (c) piezophototronic solar cells under tensile strain. The color code represents the distribution of the piezopotential at the two dimensional monolayer MoS$_2$.

Fig. 2. (a) Schematic of a monolayer MoS$_2$ piezophototronic solar cell based on the M-S contact (left side) and Ohmic contact (right side). (b) Relative current density as a function of voltage under various applied compressive strains (-0.9% to 0.9%). (c) Output power of a two-dimension MoS$_2$ piezophototronic solar cell as a function of voltage under various applied strains. (d) Open circuit voltage and maximum output power under various applied compressive strains.

Fig. 3. (a) The control ratio $\gamma$ of piezophototronic solar cell changes with $W_{piezo}$ and strain. (b) The control ratio $\gamma$ of piezophototronic solar cell increases with strain from -1% to 1% while $J_{solar}$ is 3.15 mA/cm$^2$ and 22.36 mA/cm$^2$. (c) The control ratio $\gamma$ of piezophototronic solar cell as a function of $W_{piezo}$ under applied strains of 0.2%, 0.6% and 1%. (d) The control ratio $\gamma$ of piezophototronic solar cell as a function of strain with three kinds of 2D materials: MoS$_2$, MoSe$_2$, and WSe$_2$.

Fig. 4. (a) Fill factor and (b) Power conversion efficiency of piezophototronic solar cell based on monolayer MoS$_2$ under various applied strains from -1% to 1%.
Table 1. Comparison between the Performance of Piezoelectric Solar cells Based on MoS$_2$, WSe$_2$ and MoSe$_2$.

<table>
<thead>
<tr>
<th>Materials</th>
<th>$V_{oc}$(V)</th>
<th>$J_{sc}$(mA/cm$^2$)</th>
<th>$P_{m}$(mW/cm$^2$)</th>
<th>FF$^a$</th>
<th>$V_{oc}^b$(V)</th>
<th>$P_{m}^b$(mW/cm$^2$)</th>
<th>FF$^b$</th>
<th>$\gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoS$_2$</td>
<td>0.41</td>
<td>3.15</td>
<td>0.998</td>
<td>77.30%</td>
<td>0.434</td>
<td>10.69</td>
<td>82.74%</td>
<td>0.058</td>
</tr>
<tr>
<td>WSe$_2$</td>
<td>0.82</td>
<td>17.39</td>
<td>12.29</td>
<td>86.19%</td>
<td>0.831</td>
<td>12.49</td>
<td>87.56%</td>
<td>0.014</td>
</tr>
<tr>
<td>MoSe$_2$</td>
<td>0.62</td>
<td>6.05</td>
<td>3.12</td>
<td>83.04%</td>
<td>0.640</td>
<td>3.23</td>
<td>86.21%</td>
<td>0.033</td>
</tr>
</tbody>
</table>

(a. These parameters are calculated without applied strain and b. with applied strain of 1%).

Table 2. Comparison between the Performance of Piezoelectric Solar Cells Based on MoS$_2$/InP , MoS$_2$/GaAs, MoS$_2$/Si , MoS$_2$/Graphene and MoSe$_2$/GaN.

<table>
<thead>
<tr>
<th>Materials</th>
<th>$V_{oc}$(V)</th>
<th>$J_{sc}$(mA/cm$^2$)</th>
<th>$P_{m}$(mW/cm$^2$)</th>
<th>FF</th>
</tr>
</thead>
<tbody>
<tr>
<td>MoS$_2$/InP</td>
<td>0.39</td>
<td>21.8</td>
<td>6.51</td>
<td>76.51%</td>
</tr>
<tr>
<td>MoS$_2$/GaAs</td>
<td>0.55</td>
<td>20.87</td>
<td>9.36</td>
<td>81.52%</td>
</tr>
<tr>
<td>MoS$_2$/Si</td>
<td>0.41</td>
<td>22.36</td>
<td>7.09</td>
<td>77.30%</td>
</tr>
<tr>
<td>MoS$_2$/Graphene</td>
<td>0.33</td>
<td>3.15</td>
<td>0.766</td>
<td>73.73%</td>
</tr>
<tr>
<td>MoSe$_2$/GaN</td>
<td>0.62</td>
<td>6.05</td>
<td>3.12</td>
<td>83.04%</td>
</tr>
</tbody>
</table>
Fig. 1
Fig. 2

(a) Metal MoS$_2$ Light Metal

(b) Piezo-charge $P_m$ (mW/cm$^2$)

-1.0 -0.5 0.0 0.5 1.0

0.38 0.40 0.42 0.44

(c) $P$ (mW/cm$^2$) vs. Voltage (V)

-0.9% -0.6% -0.3% 0% 0.3% 0.6% 0.9%

(d) $V_{oc}$ (V) vs. $P_m$ (mW/cm$^2$)

strain $\varepsilon$

-0.9% -0.6% -0.3% 0% 0.3% 0.6% 0.9%

$J/J_{pn0} (10^8)$

0.30 0.32 0.34 0.36 0.38 0.40

(b) $J/J_{m0} (10^8)$ vs. Voltage (V)

strain $\varepsilon$

-0.9% -0.6% -0.3% 0% 0.3% 0.6% 0.9%

$V_{oc}$ (V)

-1.0 -0.5 0.0 0.5 1.0

0.38 0.40 0.42 0.44 0.46 0.48 0.50

Fig. 2
Fig. 3

(a) 3D plot showing the relationship between strain ε (%) and piezo strain γ (%). The color bar indicates the piezo strain γ value.

(b) Graph showing the solar current density $J_{solar}$ (mA/cm²) as a function of strain ε (%). The lines represent different materials: 22.36 (MoS₂/Si), 3.15 (MoS₂/Graphene), and others.

(c) Line graph showing the relationship between piezo strain γ (%) and piezo strain γ (%) for strains ε of 1%, 0.6%, and 0.2%.

(d) Line graph showing the relationship between piezo strain γ (%) and piezo strain γ (%) for different strain ε values. The lines represent different materials: $e_{33} \times 10^{-5}$ values of 5.6 (MoS₂), 4.8 (MoSe₂), and 2.7 (WSe₂).
Fig. 4

Highlights

- Two-dimension piezo-phototronic solar cells can be a promising high-performance photovoltaic device, which have tunable properties under external applied strain.

- The piezo-phototronic effect can increase the open circuit voltage 5.8% at strain of 1%.

- The theoretical model provides a feasible structure of two dimensional piezo-phototronic solar cells for improvement of performance.