Piezophototronic Solar cell based on Third Generation Semiconductor Materials

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Abstract

By applying the outward uniform strain on the non-centrosymmetric piezoelectric semiconductor, the polarization charges on the material surface are induced. Polarization charges are often generated within the crystals provided that the applied strain is non-uniform. The strain applied has an effect on electronic transport and can be utilized to modulate the properties of the material. The effect of multiway coupling between piezoelectricity, semiconductor transport properties, and photoexcitation results in pie佐-phototronic effects. Recent studies have shown the piezoelectric and semiconductor properties of third-generation semiconductors have been used in photodetectors, LEDs, and nanogenerators. The third-generation piezoelectric semiconductor can be used in high-performance photovoltaic cells. A third-generation piezo-phototronic solar cell material is theoretically explored in this manuscript on the basis of a GaN metal-semiconductor interaction. This study aims to determine the effects of piezoelectric polarization on the electrical performance characteristics of this solar cell material. Performance parameters such as Power Conversion Efficiency, Fill Factors, I-V Characteristics, Open Circuit Voltage, and Maximum Output Power have been evaluated. The piezophototronic effect can enhance the open-circuit current voltage by 5.5 percent with an externally applied strain by 0.9 percent. The study will open a new window for the next generation of high-performance piezo-phototronic effects.
KEYWORDS: Third generation semiconductor, Piezophototronics, Piezotronics, Piezoelectricity, Solar cell

1. Introduction
Piezo-phototronics was initially proposed in 2010 [1-3]. The field of piezotronics has developed the study of the coupling between the semiconductor and piezoelectric characteristics for materials that concurrently exhibit semiconductor, photoexcitation, and piezoelectric characteristics. Also, the well-known field of optoelectronics studies the pairing of semiconductor properties with photoexcitation properties [4, 5]. The field of piezo-photonics was determined by the analysis of the linkage between piezoelectric characteristics and the characteristics of photo-excitation. The field of piezoelectric optoelectronics, which was the basis for the development of the new piezophototronics, was further developed by working on the coupling of semiconductor, photoexcitation, and piezoelectric properties [6-8]. The central feature of the piezophototronic effect is the use of piezoelectric potential to control the generation, separation, transport, and recombination processes of carriers at interfaces or junctions [1, 9]. High-efficiency optoelectronic devices, including solar cells, LEDs, and photodetectors, can be achieved by piezophototronic effects [6, 10-12].

By Comparing first-generation semiconductors, (for example, silicon, germanium) with the second-generation semiconductors, (for example, gallium arsenide, indium antimonide), the third-generation semiconductor materials such as silicon carbide (SiC), zinc oxide (ZnO), gallium nitride (GaN) and cadmium sulfide (CdS) as a rule have wider bandgap, higher thermal conductivity, greater electron saturation rate and better radiation resistance properties, and in this way attract a lot of considerations in high temperature and high-frequency applications in recent years [1, 13, 14]. The greater part of the third-generation semiconductors is wurtzite structures,
which have piezoelectric effects because of their absence of symmetry in certain directions[2, 14, 15]. These characteristics fill in as a decent scaffold for transferring mechanical stress signals between the adaptable semiconductor electronic device and the surrounding environment or the host (e.g., the human body)[16, 17].

Third generation semiconductor materials, such as GaN and SiC, distinguished by a wide band gap, have attracted considerable interest in emerging consumer electronics, 5G telecommunication technologies, automated vehicles, optoelectronics and defense technology applications owing to its superior material properties, including high voltage resistance, high switching frequency, High-temperature tolerance and high radiation resistance[18]. The wide bandgap nature and the good piezoelectric properties of these materials indicate that piezotronic and piezophototronic couplings may be important, providing excellent platforms for the analysis of the fundamental coupling between the piezoelectricity and a variety of interesting processes such as high-frequency transmission, high-field activity, and two-dimensional (2D) electron gas in associated system structures[19].

In this manuscript, we present the performance of third-generation semiconductor solar cells using a piezophototronic effect. The study model is shown below in Figure 1. A third-generation semiconductor, such as GaN, is sandwiched between two metal electrodes on the substrate as seen in Figure 1(a). One part of the metal-semiconductor-metal unit is the solar cell and the other is the electrode (ohmic contact) so it has an opposite output voltage. Polarization charges are added to the interface of the solar cell through the application of external strain as seen in Figures 1(b) and (c). The piezoelectric field raises or decreases the height of the Schottky barrier[20-22] as seen below.
2. Modulation of Piezophototronics solar cell

The theoretical models are optimized for p-n solar junction cells, and identical mathematical analyzes can be obtained for metal-semiconductor solar cells[23]. Shockley’s theory is now employed to calculate the I−V features of the piezoelectric dependent p-n junction, and evaluate the ideal p-n junction dependent on the aforementioned hypotheses: (1) the piezoelectric semiconductor has not degenerated in such a manner that the Boltzmann approximation can be implemented. (2) The piezoelectric p-n junction has an unstable depletion layer. (3) There is no generation and recombination present in the depletion layer, and the hole and electron currents are stable in the p-n junction. (4) The concentration of the dominant carrier is significantly greater than that of the minority injected. The total current density of the p-n solar cell is given by[24]:

\[
J = J_o \left[ \exp \left( \frac{qV}{kT} \right) - 1 \right] - J_{sc}
\]  

(1)

Here \( J_o \) is the saturation current, \( J_{sc} \) denotes the short-circuit current density, \( k \) stands for the Boltzmann constant, \( T \) represents the temperature, \( q \) is the elementary charge and \( V \) is the applied voltage. The saturation current can be achieved by[24]:

\[
J_o = \frac{qD_p p_{no}}{L_p} + \frac{qD_n n_{po}}{L_n}
\]  

(2)

where \( L_n \) and \( L_p \) are the diffusion lengths of holes and electrons, respectively; \( n_{po} \) and \( p_{no} \) are the electron concentration inside the p-type semiconductor and the hole concentration inside the n-type semiconductor at thermal equilibrium, respectively. Thus, the intrinsic carrier density \( n_i \) can be calculated as

\[
n_i = N_e \exp \left[ - \frac{E_g - E_{ci}}{kT} \right]
\]  

(3)
Here $E_i$ is an underlying the intrinsic Fermi level, $N_C$ is the effective density of states in the conduction band, and $E_C$ is the bottom edge of the conduction band. Without a piezo potential at the interface of the p-n junction, the relationship between the saturated current density ($J_{C0}$) and Fermi Level ($E_{F0}$) can be articulated as

$$J_{C0} = \frac{qD_p n_i}{L_p} \exp\left(\frac{E_i - E_{F0}}{KT}\right)$$  \hspace{1cm} (4)$$

The Fermi Level with piezo-potential at the interface of a p-n junction is determined by

$$E_F = E_{F0} - \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon}$$  \hspace{1cm} (5)$$

By adding equation 3, 4, and 5 the I–V characteristics of the Piezophototronic solar cell based on a third-generation semiconductor can be derived as[25]

$$J = J_o \exp\left[\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon KT}\right]\left[\exp\left(\frac{qV}{KT}\right)-1\right] - J_{sc}$$  \hspace{1cm} (6)$$

From Eqn. 6, the current transport through the p-n junction is a function of the piezoelectric charges, whose sign depends on the direction of the strain. Thus, both the magnitude and sign of the external strain (tensile or compressive) can be used to effectively adjust or control the transport current.

The open-circuit voltage ($V_{oc}$) can be evaluated by

$$V_{oc} = \frac{KT}{q} \left[\ln\left(\frac{J_{sc}}{J_{C0}}\right) + \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon KT}\right]$$  \hspace{1cm} (7)$$

The piezo-phototronic modulation ratio of the PSC can be described in terms of the open-circuit voltage and other output performance obtained from the PSC [26]:

$$\gamma = \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon KT} \ln\left(\frac{J_{sc}}{J_{C0}}\right)$$  \hspace{1cm} (8)$$
In addition, the output power is estimated as

\[
P(V) = VJ(V) \approx V \left\{ J_0 \exp\left(\frac{q^2 \rho_{\text{piezo}} W_{\text{piezo}}^2}{2 \varepsilon KT}\right) \left[\exp\left(\frac{qV}{KT}\right) - 1\right] - J_{sc}\right\}
\]  

(9)

The maximum voltage satisfies the following equation[27]:

\[
V_m + \frac{KT}{q} \ln\left(\frac{qV_m}{KT} + 1\right) = \frac{KT}{q} \ln\left(\frac{J_{sc}}{J_{co}}\right) + \frac{q^2 \rho_{\text{piezo}} W_{\text{piezo}}^2}{2 \varepsilon KT}
\]

(10)

Consequently, \( V_m \) varies with the piezoelectric charges which are induced by the applied strain \( \varepsilon \).

The maximum current density can be obtained as:

\[
J_m = J_0 \exp\left[\frac{q^2 \rho_{\text{piezo}} W_{\text{piezo}}^2}{2 \varepsilon KT}\right] \left[\exp\left(\frac{qV_m}{KT}\right) - 1\right] - J_{sc}
\]

(11)

The output maximum power \( P_m \) can be estimated as

\[
P_m = V_m J_m
\]

(12)

The fill factor can be derived from the method described in reference[28],

\[
FF = \frac{J_m V_m}{J_{sc} V_{oc}} \approx \frac{P_m}{J_{sc} V_{oc}}
\]

(13)

The power conversion efficiency (PCE) is defined in [22, 28]:

\[
PCE = \frac{J_{sc} V_{oc} FF}{P_m}
\]

(14)

3. Result and Discussion

Typical constants are utilized in computations of the performance parameters such as the \( \text{Voc}, \ P_m, \ \text{PCE}, \text{and FF} \). The temperature was assigned at 300K, \( W_{\text{piezo}} \) is thought to be 0.543 nm [29], the relative dielectric constant of GaN is 8.9 [30], and \( e_{33} \) of the GaN is estimated to be 0.73 C/m² [31].

The relative current density \( J/J_{pn0} \) versus voltage (\( J/J_{pn0} \)-V curve) of the GaN PSC with the external strain varying in the range of -0.9% to 0.9% When the short circuit current \( J_{sc} \) is taking to be 4.4
mA/cm$^2$[32] is plotted in Figure 2(a). Figure 2(b) shows the PCE of piezoelectric solar cells based on different types of materials at an external strain of 0.9%, indicating that the J increases with the strain and peaks at Vm. By employing equation (13) and equation (14), the Fill Factor (FF) and power conversion efficiency (PCE) parameter which aid in explaining the characteristics and performance of PSC is illustrated in Figure 2(c) and (d). The FF is linearly dependent on the externally applied strain between the regions -0.9% to 0.9 with a step of 0.3%. The improvement in FF can be credit to the increased Voc when is under strain. The PCE and modulation ratio ($\gamma$) considered in Figure 2 (b) and (c) is determined by utilizing similar parameters as in GaN such as $J_{sc}$, $J_{pno}$, etc, at an applied strain of 0.9% and 1% respectively. The different parameters utilized are the piezoelectric constant and the relative dielectric constant. The piezoelectric constant and relative dielectric constant are given in Table 1.1. The PCE and modulation ratio ($\gamma$) of AlN is observed to increase more distinctly than GaN and ZnO within the strain region of 0.9 and 1% respectively. This can be attributed to the large piezoelectric constant and small relative dielectric constant of AlN material. By considering the impact of material properties, the ratio of piezoelectric constant to that of relative dielectric constant plays an essential part in the performance of PSC[33,34]. Among the third-generation semiconductor materials, the AlN has a noteworthy modulation ratio of 9.3% follows by ZnO (7.96%) and GaN (4.78%). The modulation ratio of AlN happens to be almost twice greater than GaN. The superior performance of AlN, ZnO, and GaN is due to the large piezoelectric constant, this demonstrates that a good performing material is the one with a large piezoelectric constant and small relative dielectric constant.

Figure 3(a) and (b) show the graph of maximum power (Pm) and open-circuit voltage (Voc) against applied external strain. By utilizing Equation (7) and Equation (12), the Voc and Pm are linearly identifying with the strain(s). By introducing the piezo-phototronic effect, the performance
parameters of the GaN PSC improve due to enhancement in Vm and Pm. The modulation ratio for GaN PSC as against W_{piezo} as a function of strain is illustrated in Figure 3(c). As the width of the piezo-charge opens up the modulation ratio also increases. Furthermore, the modulation ratio is linearly dependent on both the external applied strain and W_{piezo}. The semiconductor material and metal contact can influence W_{piezo}[35, 36]. The piezoelectric constant and their dielectric constant of different third-generation semiconductor materials are plotted in Figure 3(d).

4. Summary

The idea of piezophototronic enhanced third-generation semiconductor material solar cells has been proposed and hence reenacted in this work. Key performance parameters portraying the device including Voc, Pm, P, and FF have been mathematically determined. It is indicated that the PSC shows an enhanced performance under externally applied strains, especially for the modulation ratio. Additionally, GaN, ZnO, and AlN show a more prominent potential for high-efficiency PSCs. This gives physical insights into the PSCs and can serve as guidance on the design of third generation piezo-phototronic energy harvesting devices.

Conflict of interest

The authors declare that they have no conflict of interest

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Author contribution statement

All authors have been contributed equally

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Table 1:1 shows the piezoelectric constant and relative dielectric constant.
| Material(s) | Piezoelectric constant $e_{33} (C/m^2)$ | Relative dielectric constant |
|-------------|----------------------------------------|----------------------------|
| GaN        | 0.73[31]                               | 8.9[30]                    |
| AlN        | 1.46[37]                               | 9.14[38]                   |
| InN        | 15.3[37]                               | 0.97[30]                   |
| InAs       | 15.15[37]                              | -0.03[39]                  |
| ZnO        | 1.22[40]                               | 8.92[40]                   |
| CdS        | 5.7[41]                                | 0.44[42]                   |
| CdSe       | 5.8[41]                                | 0.347[43]                  |
| CdTe       | 11[37]                                 | 0.03[44,45]                |

**Figure Captions**

Figure 1 Schematic structure and energy band configuration of third generation PSC semiconductor material (GaN). (a) Without strain; (b) with tensile strain; (c) with compressive strain;

Figure 2 (a). Relative current density-voltage ($J/J_{p00}$-V) curve with Strain ($\varepsilon$) increasing in the range of [-0.9% 0.9%]. (b) Comparative analysis of PCE for piezoelectric solar cell based on different types of materials with an external strain of 0.9%. (c) $\gamma$ of the various types of piezoelectric solar cells material under an applied strain of 1% and (d) FF of GaN PSC with the applied strain varying in the region [-0.9% 0.9%]

Figure 3 (a) $P_m$ and (b) $V_{oc}$ versus the external strain applied. (c) Modulation ratio $\gamma$ of the GaN PSC with $W_{piezo}$ under the strain ($\varepsilon$) of 0.3% 0.6% and 1%. (d) The piezoelectric constant of various third-generation semiconductor materials as opposed to their various dielectric constant.
Figures

(a) Unstrained
(b) Compressed
(c) Stretched

Figure 1
Figure 2
Figure 3