

ENHANCED THIRD GENERATION SEMICONDUCTOR MATERIAL-BASED SOLAR CELL EFFICIENCY BY PIEZO-PHOTOTRONIC EFFECT[†]

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Received January 20, 2022; accepted March 16, 2022

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 piezo-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: Polarization charges; Piezophototronic effect; Solar cell; third-generation semiconductor; piezoelectric effect.

PACS: 42.79.Ek; 42.70.Nq

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 photo-excitation 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 semiconductors, photo-excitation, and piezoelectric properties [6,7]. 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 bandgap, have attracted considerable interest in emerging consumer electronics, 5G telecommunication technologies, automated vehicles, optoelectronics, and defense technology applications owing to their superior material properties, including high voltage resistance, high switching frequency, High-temperature tolerance and high radiation resistance [16]. 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 [17]. Currently, ZnO has undergone extensive research as a candidate material for piezophototronic-based solar cells, but little is known about piezoelectric GaN and AlN. This paper could be used to fill this knowledge gap.

[†] Cite as: M. Gyan, J. Parbby, and F.E. Botchey, East. Eur. J. Phys. 1, 70 (2022), <https://doi.org/10.26565/2312-4334-2022-1-10>
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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.

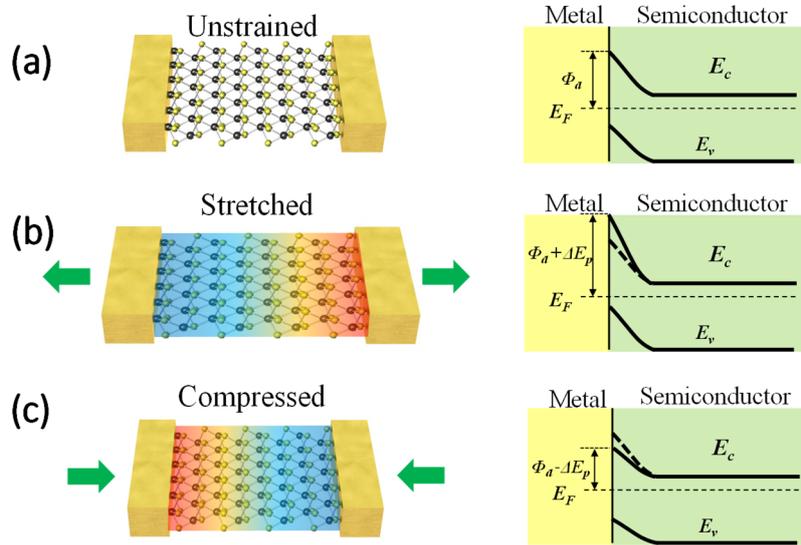


Figure 1. Schematic structure and energy band configuration of third-generation PSC semiconductor material (GaN). (a) Without strain; (b) with tensile strain; (c) with compressive strain;

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 [20]. Polarization in semiconductor can be taken into account by expressing it as [21]

$$D = \epsilon_o \epsilon_r E + P \tag{1}$$

Where D is electric displacement, ϵ_o and ϵ_r are vaccum and relative permittivities respectively E is electric field and P is the total polarization.

Hook’s law can be use to describe the association between the polarization and a small form of mechanical strain and this is expressed by [22,23,24]

$$P = e_{ijk} S_{jk} \tag{2}$$

Where S is mechanical strain, e_{ijk} is the piezoelectric tensor (third order tensor). For a semiconductor grown along c-axis with the strain component S_{33} , the polarization P is expressed by

$$P = -e_{33} S_{33} = q \rho_{piezo} W_{piezo} \tag{3}$$

The poisson equation describes the electrostatic behavior of charges within semiconductor materials

$$\nabla^2 V = -\rho / \epsilon \tag{4}$$

Where V is the potential, ϵ is the permittivity of the material and P is the charge density.

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 [22]:

$$J = J_o \left[\exp\left(\frac{qV}{KT}\right) - 1 \right] - J_{sc} \tag{5}$$

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 [22]:

$$J_o = \frac{qD_p p_{no}}{L_p} + \frac{qD_n n_{po}}{L_n} \quad (6)$$

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

$$n_i = N_c \exp\left[-\frac{E_c - E_i}{KT}\right] \quad (7)$$

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_{co}) and Fermi Level (E_{Fo}) can be articulated as

$$J_{co} = \frac{qD_p n_i}{L_p} \exp\left(\frac{E_i - E_{Fo}}{KT}\right) \quad (8)$$

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

$$E_F = E_{Fo} - \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\epsilon_s} \quad (9)$$

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]

$$J = J_o \exp\left[\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\epsilon_s KT}\right] \left[\exp\left(\frac{qV}{KT}\right) - 1\right] - J_{sc} \quad (10)$$

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

$$V_{oc} = \frac{KT}{q} \left[\ln\left(\frac{J_{sc}}{J_{co}}\right) + \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\epsilon_s KT} \right] \quad (11)$$

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]:

$$\gamma = \frac{\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\epsilon_s KT}}{\ln\left(\frac{J_{sc}}{J_{co}}\right)} \quad (12)$$

In addition, the output power is estimated as

$$P(V) = VJ(V) \approx V \left\{ J_o \exp\left(\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\epsilon_s KT}\right) \left[\exp\left(\frac{qV}{KT}\right) - 1\right] - J_{sc} \right\} \quad (13)$$

The maximum voltage satisfies the following equation [27]:

$$V_m + \frac{KT}{q} \ln\left(\frac{qV_m}{KT} + 1\right) = \frac{KT}{q} \left[\ln\left(\frac{J_{sc}}{J_{co}}\right) + \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\epsilon_s KT} \right] \quad (14)$$

Consequently, V_m varies with the piezoelectric charges which are induced by the applied strain ϵ . The maximum current density can be obtained as:

$$J_m = J_o \exp\left[\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\epsilon_s KT}\right] \left[\exp\left(\frac{qV_m}{KT}\right) - 1\right] - J_{sc} \tag{15}$$

The output maximum power P_m can be estimated as

$$P_m = V_m J_m \tag{16}$$

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

$$FF = \frac{J_m V_m}{J_{sc} V_{oc}} \approx \frac{P_m}{J_{sc} V_{oc}} \tag{17}$$

The power conversion efficiency (PCE) is defined in [19,28]:

$$PCE = \frac{J_{sc} V_{oc} FF}{P_{in}} \tag{18}$$

RESULT AND DISCUSSION

Typical constants are utilized in computations of the performance parameters such as the V_{oc} , P_m , PCE, and FF. The temperature was assigned at 300K, W_{piezo} is thought to be 0.543 nm [29], the relative dielectric constant of GaN is 8.9 [30], and ϵ_{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/cm²[32] is plotted in Figure 2(a).

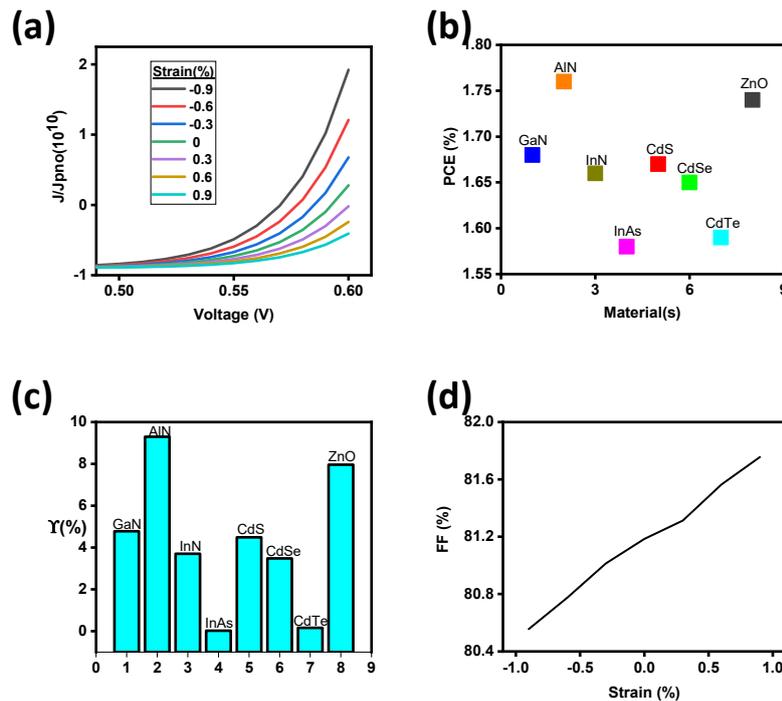


Figure 2. (a). Relative current density-voltage (J/J_{pn0} -V) curve with Strain (ϵ) increasing in the range of [-0.9% 0.9%]. (b) Comparative analysis of PCE for piezoelectric solar cell based on different types of materials with an external strain of 0.9%. (c) modulation ratio (γ) of the various types 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 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 V_m . By employing equation (17) and equation (18), 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 credited to the increased V_{oc} when it is under strain. The PCE and modulation ratio (γ) considered in Figure 2 (b) and (c) is determined by utilizing similar parameters as in GaN such as J_{sc} , J_{pn0} , 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. The PCE and modulation ratio (γ) 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 (11) and Equation (16), 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).

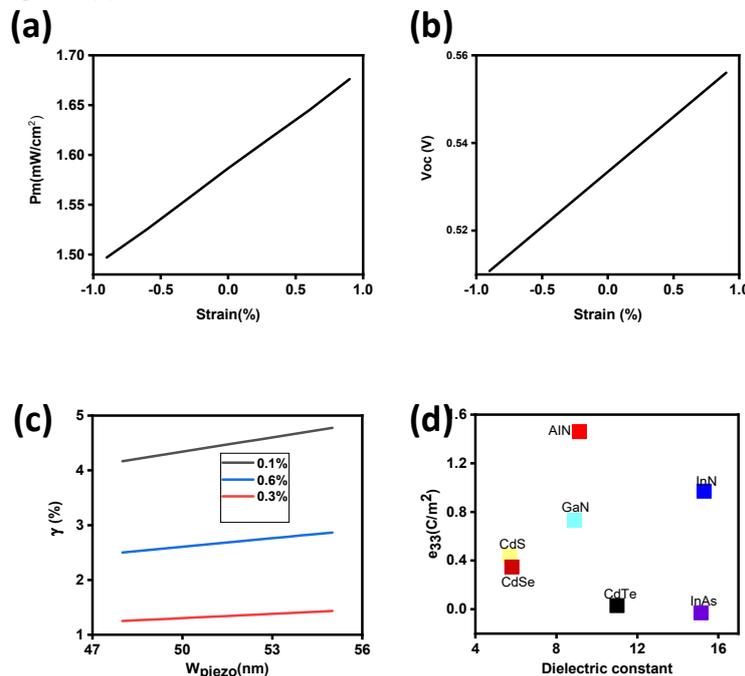


Figure 3. (a) Pm and (b) Voc versus the external strain applied. (c) Modulation ratio γ of the GaN PSC with W_{piezo} under the strain (ϵ) of 0.3% 0.6% and 1%. (d) The piezoelectric constant of various third-generation semiconductor materials as opposed to their various dielectric constant.

Table 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]

SUMMARY

In conclusion, we investigated the properties of a strained photovoltaic Schottky contact metal/semiconductor PV solar cell and examined the piezo-phototronic effect produced in the junction when the PV cell was strained. The piezoelectric effects in this structure are thought to be caused by external applied mechanical stress. 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.

Funding. This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

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**ПІДВИЩЕННЯ ЕФЕКТИВНОСТІ СОНЯЧНИХ ЕЛЕМЕНТІВ ТРЕТЬОГО ПОКОЛІННЯ
НА ОСНОВІ П'ЄЗО – ФОТОТРОННОГО ЕФЕКТУ
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Прикладаючи зовнішню рівномірну деформацію на нецентросиметричний п'єзоелектричний напівпровідник, індуються поляризаційні заряди на поверхні матеріалу. Поляризаційні заряди часто генеруються всередині кристалів за умови, що прикладена деформація нерівномірна. Застосована деформація впливає на електронний транспорт і може бути використана для модуляції властивостей матеріалу. Ефект багатостороннього зв'язку між п'єзоелектрикою, властивостями перенесення напівпровідників і фотозбудженням призводить до п'єзо-фототронних ефектів. Останні дослідження показали, що п'єзоелектричні та напівпровідникові властивості напівпровідників третього покоління використовуються у фотодетекторах, світлодіодах та наногенераторах. П'єзоелектричний напівпровідник третього покоління можна використовувати у високоефективних фотоелементах. У цій роботі теоретично досліджується матеріал п'єзофототронного сонячного елемента третього покоління на основі взаємодії металу та напівпровідника GaN. Це дослідження спрямоване на визначення впливу п'єзоелектричної поляризації на електричні характеристики цього матеріалу сонячних елементів. Були оцінені такі експлуатаційні параметри, як ефективність перетворення потужності, коефіцієнт заповнення, I-V характеристики, напруга розімкнутого ланцюга та максимальна вихідна потужність. П'єзофототронний ефект може підвищити напругу струму разомкнутого ланцюга на 5,5 відсотка при зовнішній деформації на 0,9 відсотка. Дослідження відкриє нове вікно для наступного покоління високоефективних п'єзо-фототронних ефектів.

Ключові слова: поляризаційні заряди; п'єзофототронний ефект; сонячна панель; напівпровідник третього покоління; п'єзоелектричний ефект