Nano Energy (2015) 14, 257–275

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/nanoenergy

Fundamental theories of piezotronics and piezo-phototronics

Ying Liu[a], Yan Zhang[a,b], Qing Yang[a], Simiao Niu[a], Zhong Lin Wang[a,b,*]

[a]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0245, United States
[b]Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing, 100083, China

Received 8 October 2014; received in revised form 14 November 2014; accepted 25 November 2014
Available online 3 December 2014

KEYWORDS
Piezotronic effect;
Piezo-phototronic effect;
LED;
Solar cell

Abstract
Wurtzite structured mateirals such as ZnO, GaN, InN and CdS simultaneously exhibit piezoelectric, semiconducting and photoexcitation properties. The piezotronic effect is to use the inner crystal potential generated by piezoelectric polarization charges for controlling/tuning the charge carrier transport characteristics in these materials. The piezo-phototronic effect is about the use of piezoelectric charges to tube the generation, transport, separation and/or recombination of charge carriers at p-n junction. This article reviews the fundamental theories of piezotronics and piezo-phototronics, forming their basis for electromechancial devices, sensors and energy sciences. Starting from the basic equations for piezoelectricity, semiconductor and photoexcitation, analytical equations for describing the strain-tuned device current were derived. Through analytical calculations and numerical simulations, it was confirmed that the piezoelectric polarization charges can act in the form of inner-crystal charges in the depletion region, resulting in a change in Schottky barrier height, depletion region shift and/or formation of a charge channel, which can be used effectively to enhance the efficiency of LED, solar cell and photon detectors.

Introduction

Piezoelectric materials have a wide range of applications in sensors, actuators and energy harvesting. In recent years, much attention has been focused on piezoelectric semiconductor materials in the Wurtzite family, such as ZnO, GaN, InN and CdS [1-7]. Due to the coupling of piezoelectric, semiconducting and photoexcitation properties, as shown in Fig. 1, the new fields of piezotronics and piezo-phototronics have been created. The piezotronic effect is to use the inner crystal potential generated by piezoelectric polarization charges for controlling/tuning the charge carrier transport characteristics and fabricating mechanical-electronic devices. Such devices

*Corresponding author at: School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia 30332-0245, United States
E-mail address: zlwang@gatech.edu (Z.L. Wang).

http://dx.doi.org/10.1016/j.nanoen.2014.11.051
2211-2855/

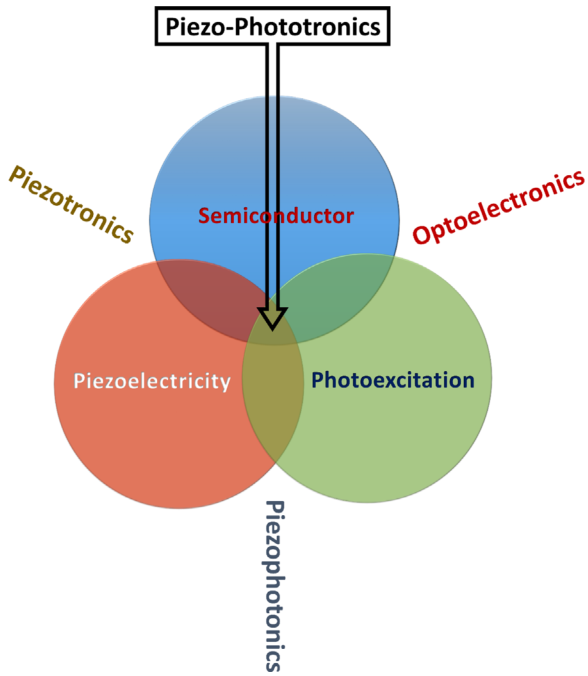

Fig. 1 Schematic diagram showing the three-way coupling among piezoelectricity, photo excitation and semiconductor properties.

can be the basis for active flexible electronics, which uses the mechanical actuation from the substrate for inducing new electronic/optoelectronic effects, with potential applications in micro-electromechanical systems, nanorobotics, human-computer interfacing and sensors [8]. The piezo-phototronic effect is about the use of piezoelectric polarization on the generation, transport, separation and/or recombination of charge carriers at p-n junction, in devices including photocells, photodetectors and LEDs, their performances and interaction with light are significantly changed by externally applied strain [9-11].

Since year 2008, abundant experimental studies have been reported to demonstrate the existence of the piezotronic and piezo-phototronic effects in ZnO, GaN and other Wurtzite structured material based devices [10-17]. In all these reports, several common phenomena are discovered: (i) strain can monotonically tune the device current; (ii) the change of device current switched polarity with the polarity of applied strain or direction of c-axis; (iii) photoresponse and photoemission can be dramatically enhanced by strain, and the enhancement of photoemission is much greater than the change of current; (iv) in devices with one p-n junction or Schottky junction on each end of the nanowires, asymmetric changes between positive biased current and negative biased current were recorded. To explain these observations, theoretical study will not only provide an in-depth understanding about these results, but also explore the core factors in this effect and build high performance devices.

Thus, from 2011, numerous theoretical analysis and numerical simulations have been performed to investigate the physics mechanisms behind the experimental results [18-20]. Starting from coupling the basic equations of piezoelectricity, semiconductor physics and photoexcitation, analytical equations of piezotronics and piezo-phototronics were derived. Specifically, the current-voltage characteristics of piezotronics/piezo-phototronics devices were expressed as functions of applied strain. The tuning effect of piezoelectric polarization was revealed in the relationship between device performance and mechanical deformation. Numerical simulations including Finite Element Method were then used to verify the analytical theory. Numerically simulated band structures confirmed the assumptions and conclusions from the analytical study. Taking into consideration the unideal factors, device current of both one-dimensional (1D) devices and two-dimensional (2D) devices were simulated and compared over strain range used in experiments, which intuitively demonstrated how the mechanism revealed could influence device performance, as well as extrapolate the basic theory into optimization methodology for future device designs. This review is intended to give a comprehensive coverage of the theoretical work done in piezotronics and piezo-phototronics in order to illustrate their fundamental understanding and intrinsic physics.

Theory of piezotronics [20]

Analytical solution for one-dimensional simplified p-n junction

The nature of piezotronics lies in the tuning effect of piezoelectric polarization on semiconductor behaviors. In most of the semiconductor devices, the formation of junctions at material interface is usually the essential part for realizing function of the device. Junction area is also where piezoelectric charges (piezo-charges) accumulate. The piezotronics effect could be evaluated by how strain tunes the current characteristics in devices such as a piezotronic sensor.

In piezotronics, the fundamental governing equations for both semiconductor and piezoelectric theories included electrostatic equations, current-density equations, continuity equations, [21] and the piezoelectric equations [22].

1) The Poisson equation is the basic equation for describing the electrostatic behavior of charges

$$\nabla^2\psi_i = -\frac{\rho(\vec{r})}{\varepsilon_s} \tag{1}$$

where ψ_i is the electric potential distribution and $\rho(\vec{r})$ is the charge density distribution, and ε_s is the permittivity of the material.

2) The current-density equations that correlate the local fields, charge densities and local currents are

$$\begin{cases} \vec{J}_n = q\mu_n n\vec{\mathbf{E}} + qD_n\vec{\nabla}n \\ \vec{J}_p = q\mu_p p\vec{\mathbf{E}} - qD_p\vec{\nabla}p \\ \vec{J}_{\text{cond}} = \vec{J}_n + \vec{J}_p \end{cases} \tag{2}$$

where $\vec{J}_n$ and $\vec{J}_p$ are the electron and hole current densities, q is the absolute value of unit electronic charge, μ_n and μ_p are electron and hole mobilities, n and p are concentrations of free electrons and free holes, D_n and D_p are diffusion coefficients for electrons and holes, respectively, E is electric field, and $\vec{J}_{\text{cond}}$ is the total current density.