



An accurate computational method for analysis of electromechanical properties of structures with metal-GaN piezoelectric semiconductor contact

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ABSTRACT

An accurate computational method is proposed to analyze the electromechanical characteristic of structures of metal-piezoelectric semiconductor contact based on the nonlinear theory of piezoelectric semiconductors. In this method, two boundary value problems (BVPs) are solved iteratively. One is called the mechanical BVP, and the other is the semiconductor BVP. Piezoelectricity is used to link these two BVPs. The piezoelectric polarization charges are deeply taken into account in the bidirectional coupling of mechanical field and semiconductor. An experimental configuration is designed to determine the contact type, that is, Schottky contact or Ohmic contact. At the same time, the iterative method based on the commercial software COMSOL is employed to analyze this configuration numerically. A validation of the algorithm is conducted by comparing the experimental and numerical results. As an application, the electromechanical properties of a typical Ag-GaN piezoelectric semiconductor structure are investigated by the developed approach. The results revealed that it can be totally applied to analyze and predict the electromechanical properties of semiconductor materials with piezoelectricity.

1. Introduction

In recent years, much attention has been focused on the material properties of the Wurtzite family, such as GaN and ZnO [1–5]. Owing to the coupling piezoelectric and semiconducting properties, this type of material is called a piezoelectric semiconductor (PSC) [6,7]. As a new kind of smart electronic material with piezoelectric-semiconductive effect, PSCs have been widely used in various multi-functional and electromechanical devices [8–11], and the properties have been studied increasingly intensively. For example, Yang et al. [9] analyzed the effects of semiconduction on electromechanical energy conversion in piezoelectrics. Wang et al. [12] discussed the coupling effect between piezoelectric and semiconducting properties which led to the creation of the new field of “piezotronics”.

As is well-known, electronic devices are connected to the external circuit by metal electrode, where the bias voltage is applied [13]. So the metal-semiconductor contact is an important component in electronic devices [14]. For PSCs, due to the coupling of piezoelectricity and conductivity, the structures with metal-piezoelectric semiconductor (M-PSC) contacts exhibit many special properties. Mechanical deformation can produce piezoelectric polarization charges and induce the

movement of free charges [15]. The inner crystal potential generated by piezoelectric polarization charges can be used for controlling/tuning the carrier transport characteristics of PSC devices. Based on the special properties, Wang [16] reviewed the fundamental theories of a metal-ZnO nanowire contact, analyzed the piezoelectric polarization charges at the interface of a junction and studied the effect of the piezoelectric polarization charges on the carrier transport characteristics of ZnO devices. Araneo et al. [17] investigated the charge transport behavior in ZnO nanowires under uniaxial loading. The surface piezoelectric polarization charges that appeared at the metal-semiconductor contacts were assumed to be distributed within a maximum distance δ_{piezo} , and this distance was regarded as a key parameter that affects the I - V characteristics of piezosemiconductive devices.

Although a few of impressive research efforts have been performed [18–22], some key issues concerning the electromechanical characteristics of PSC structures and devices are still challenging from both a physical and computational point of view. Up to now, there is no effective tool to analyze the coupling performances of PSC structures especially under the combined electrical and mechanical loading. In the previous numerical simulations [16,17], the piezoelectric equations and the semiconductor equations were enforced introduced into the

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PDE module of COMSOL Multiphysics software to calculate the electromechanical properties of PSC. In order to establish the coupling of piezoelectricity and semiconductor properties, many assumptions were made. For example, the piezoelectric polarization charges were assumed to be uniformly distributed in the metal-semiconductor junction and the distributed width (W_{piezo}) was proposed to be 0.25 nm. Especially, the density of the polarization charges was obtained from the piezoelectric-semiconductive effect directly calculated by assuming that the PSC material was an insulator. And the distribution field of piezoelectric polarization charges was preloaded into the model before structure analysis. The used parameters and assumptions were physically groundless. Therefore, the obtained results, for example, the influence of the distribution on the current-voltage (I - V) characteristics of the structure, were inconvincible. It should be noted that all fields, including the mechanical and electrical fields, and the distribution of piezoelectric polarization charges in the PSC structures should be coupled and are unknown before solution. Therefore, a rigorous analysis method is urgently needed in this area to design and analyze the electromechanical characteristics of M-PSC structures.

Zhao et al. [23] proposed a piezoelectric-conductor iterative method by using the commercial software ANSYS and the elements for a piezoelectric media and conductor based on the linearized theory. However, many nonlinear characteristics cannot be simulated or predicted based on linear theory.

Motivated by the above issues, in this paper, a computational method is proposed for the full analysis of the M-PSC structures based on the nonlinear equations of PSC, in which all physical fields are coupled and obtained without any assumption. The effects of the piezoelectric polarization charges on the performance of electric transport of M-PSC heterojunction are deeply analyzed. The paper is organized as follows. Following the introduction, the measurement configuration of the contact type of Ag-GaN and the experiment are presented in Section 2. The experimental results are used to validate the proposed analysis method. In Section 3, an iterative method for analysis of PSC structures is developed. In Section 4, the electromechanical properties of a typical M-PSC contact structure are analyzed by using the proposed method. Finally, the conclusions are proied in Section 5.

2. Determination for the contact type of M-PSCs

To study and predict the electromechanical characteristics of the structures of M-PSCs, we first need to know the contact type, that is, the electrical boundary conditions. For example, according to Schottky theory [24], for n-type semiconductors, when the metal work function is greater than the semiconductor work function, the contact type is the Schottky contact, otherwise, it is the Ohmic contact. To clarify the contact type of M-PSCs, an experimental configuration was designed. At the same time, the experimental configuration provided a benchmark to test and validate the analytical and numerical methods and solutions.

Fig. 1 shows a schematic of the experimental configuration for the measurements of the I - V characteristics of M-PSC structures. To make the samples insulated from the bracing structure, the specimen was placed on the Polytetrafluoroethylene (PTFE) sheet. Two probes were used to contact the electrode and the semiconductor surface, respectively. A pre-stress of 5 MPa was applied by a mechanical spring to ensure that the probe was closely connected to the contact surface.

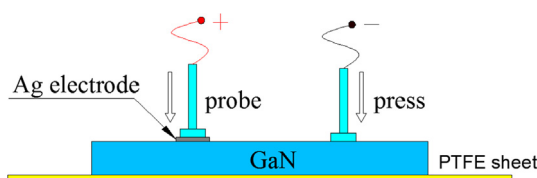


Fig. 1. Schematic representation of experimental configuration for the measurement of the contact type of Ag-GaN.

GaN, as a new kind of electronic material, exhibits excellent functional properties in microwave devices, such as direct bandgap, high breakdown voltage, high saturation velocity, and high thermal stability [25–28]. Hence, GaN was used as the test material in the present paper. The pure GaN material shows an n-type semiconductor property. The dimensions of the smooth-rectangular-plate samples in the present work are shown in Fig. 1, with a length 20.0 mm, width 10.0 mm, and thickness 2.0 mm. The surface roughness of the sample was 0.2 μm .

The work function of elemental silver is 4.26 eV [29], while the work function of GaN has been reported as 4.2 eV in Ref. [30] and 4.3 eV in Ref. [31]. In practical applications, the used electrodes are not made from pure silver and may contain other elements. Thus, the actual metal-semiconductor contact surface is usually not ideal. The contact type can vary with physical conditions [24,32]. Therefore, it is difficult to judge the contact type of the Ag-GaN structure theoretically.

To eliminate the impurities that are introduced by processes such as physical adsorption and chemical adsorption, the specimens were cleaned by ultrasonic waves in acetone solution for 5 min, and then the contact surface was corroded by hydrogen peroxide. After that, the specimens were rinsed with deionized water, dried by nitrogen, and baked in a dry oven at 90 $^{\circ}\text{C}$ for 5 min. Finally, the silver electrode was plated and sintered on the contact position.

Ten specimens were measured and all tests were conducted at room temperature. The test results are shown in Fig. 2. It can be seen that when an external voltage was applied on the left-hand probe with a positive bias, a forward current from the metal to the semiconductor was developed. The current was exponentially changed with the increase of the voltage. When a negative bias was applied, a reverse current from the semiconductor to metal was developed. However, the reverse current was very small and had little or nothing to do with the reverse voltage. The results demonstrate that the contact type of Ag-GaN PSC in the present paper was a Schottky contact.

3. Iterative method for analysis of M-PSC structures

3.1. Governing equations

To describe the characteristics of M-PSCs, it is necessary to start from a consistent physical mathematical model. The classical approach [33–38] was successfully applied in practice and a system of fully coupled nonlinear partial differential equations was derived to describe the mechanical deformation, the charge transport and the electrical behavior of the devices.

The mechanical elastic behavior of PSCs is governed by Newton's law [39].

$$\sigma_{ij,j} = 0, \quad (1)$$

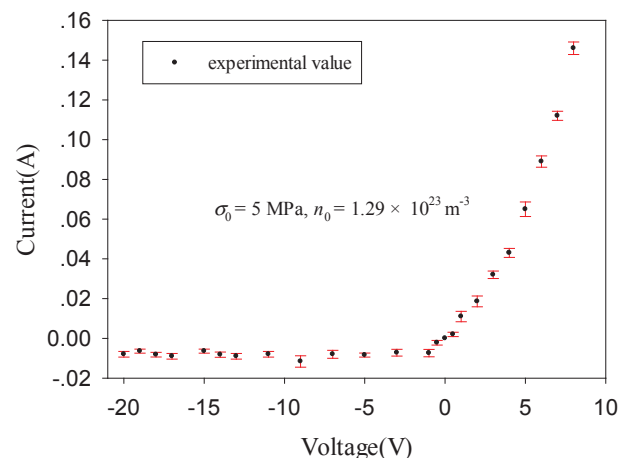


Fig. 2. The measured I - V characteristics.

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