Nano Energy (▮▮▮▮) ▮, ▮▮▮–▮▮▮

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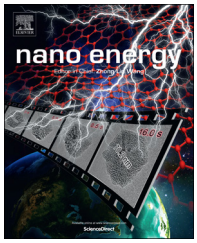

First principle simulations of piezotronic transistors

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Received 4 September 2014; received in revised form 30 September 2014; accepted 2 October 2014

KEYWORDS
Piezotronic transistor;
First principle simulations;
Width of piezoelectric charge distribution;
Modulation of Schottky barriers

Abstract
Piezoelectric semiconductors, such as wurtzite structured ZnO, GaN, and InN, have novel properties owing to piezoelectric polarization tuned/controlled electronic transport characteristics. Under an externally applied strain, piezoelectric charges are created at an interface or junction, which are likely to tune and modulate the local band structure. Taking an Ag-ZnO-Ag two-terminal piezotronic transistor as an example, strain-dependent piezoelectric charge distributions and modulation of Schottky barrier heights (SBHs) at metal/semiconductor interfaces have been investigated by the first principle simulations. The width of piezocharge distribution is calculated by the density function theory and the Poisson equation. The modulations of SBHs at two interfaces show opposite trend under the applied strain. This study not only provides an understanding about the piezotronic effect from quantum theory point of view, but also a new method to calculate the key parameter for optimizing the design of piezotronic devices.

Introduction

Piezoelectric semiconductor materials, such as wurtzite ZnO, GaN, InN, and CdS, have drawn intensive research interests for fabricating functional electronics [1-3]. Under an externally applied mechanical strain, piezoelectric charges (piezocharges) are created at a metal-semiconductor interface or a *pn* junction, which are likely to tune the local Schottky contact or charge-depletion zone and can be used as a new means for "gating" carrier transport. This is a new emerging field of piezotronics [4]. Piezotronic effect has been studied and utilized for two-terminal strain gated transistors [5,6], logic devices [7], memory units [8], enhancing solar cell and LED efficiency [9,10], enhanced gas/chemical/bio-sensing [11-13], and straining mapping [14]. Recently, array and chip based piezotronic devices have been developed as flexible human-machine interfacing [15]

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http://dx.doi.org/10.1016/j.nanoen.2014.10.014
2211-2855/

and photonic-strain mapping [16], setting a milestone from fabricating single devices to an array of devices and even to an integrated system [17].

Theoretical studies have been carried to understand the fundamentals of piezotronics using semi-classical models, including piezopotential distribution in strained ZnO nanowires [18,19], the influence of piezopotential spatial distribution on local contact dictated transport properties of ZnO nanowires [20], and the establishment of theoretical framework of piezotronics for qualitative understanding carrier transport behavior [21]. Recently ab initio simulations studies are employed to investigate the piezoresistance effect with the change in bandgap under strain for the nanoscopic transistor [22,23]. Piezoresistance effect is a volume based effect without polarity that is a common feature for almost any semiconductors. However, piezotronic effect is a result of piezoelectric charges at the local interface that has strong polarity dependence, thus, exhibiting an asymmetric or non-symmetric effect on the local contacts at the ends of a wurtzite or zinc-blende structured material. From our previous theoretical work [21], the width of piezoelectric charge distribution at the local interface is an important factor for piezotronics, but such information cannot be provided by the classical piezotronic theory although we believe that the charge distribution is within a few atomic layers. The ab initio methods are computational methods from first principles of quantum mechanics, and used for calculating atomic and molecular structure based entirely on quantum mechanics and basic physical constants. Density functional theory (DFT) method is one of the most important ab initio methods for calculating molecules electronic structure. DFT simulation can provide quantitative information about the width of piezoelectric charges at the interface and their distributions depending on the piezoelectric semiconductor material and crystal structure.

In this article, we present the first ab initio calculation on the piezotronic effect in a metal-semiconductor-metal based two-terminal piezotronic transistor. The distribution of piezoelectric charge density at the metal-semiconductor interface is investigated and its influence on the local Schottky barrier height is studied. By using the density functional theory, the electrostatic potential within the transistor can be obtained. Then the Poisson equation is employed to calculate the charge density from the electrostatic potential. Based on the charge density, the piezoelectric charge distribution and the total piezoelectric charge versus strain are calculated. Furthermore, the modulation of Schottky barrier height by the piezotronic effect is calculated in the interface region under the strain. Our study provides the first quantum mechanical understanding about piezotronic effect and establishes its physics bases starting from first principle. This study is important for quantitative understanding the effect and optimized design of piezotronic devices.

Model and method

To illustrate the first-principles calculations based on the DFT simulation for the piezotronics, a typical metal-semiconductor-metal (MSM) piezotronic transistor is taken as an example. Figure. 1 shows an Ag-ZnO-Ag transistor, including the center ZnO sandwiched between the left-hand and right-hand side Ag electrodes. In our model, ZnO has a hexagonal wurtzite structure, with its *c*-axis chosen pointing from the left to the right Ag electrode, as shown in Figure. 1. The Ag(1 1 1) plane is assumed to directly interfacing with the $\pm$(0001) polar planes of ZnO. The atomic structure of ZnO and Ag are also given in Figure. 1: the white ball denotes to Zn atom, red ball for O atom, and blue ball for Ag atom. According to the classical piezotronics theory, when a tensile strain along the *c*-direction is applied on the transistor, negative piezoelectric charges are created at the $-c$ side of the metal-semiconductor (M-S) interface (ZnO(000$\bar{1}$)-Ag junction), while positive charges are created at the $+c$ side (ZnO(0001)-Ag junction). Alternatively, the signs of charges reverse when a compressive strain is applied. Positive piezoelectric charges induce positive piezoelectric potential and lower the barrier height at the local contact, while negative charges induce negative potential and raise the barrier height.

A lateral view of the Ag-ZnO-Ag piezotronic transistor is shown in Figure. 2(a) without applying strain. In the present study, the transistor consists of four double (eight single) Zn-O layers as center region and Ag(1 1 1) layers on the left-hand (000$\bar{1}$) and right-hand (0001) side of ZnO, respectively, as two electrodes. ZnO{0001} direction and Ag(1 1 1) plane parallel to *c* axis and *a*-*b* plane of the transistor supercell, respectively. Four planes represented by black dashed lines in parallel to Ag(1 1 1) plane, A, B, C, and D, divide the transistor into three regions: AB is the left-hand electrode contacting to ZnO(000$\bar{1}$)-O polar surface, CD is the right-hand one contacting ZnO(0001)-Zn polar surface, and BC is the center ZnO region [24]. The periodical boundary condition is applied to all *a*, *b*, and *c* directions of the supercell; the box in Figure. 2(a) shows the supercell of the transistor used for the calculation. For simplicity, we neglect the effect of impurity/defect in our transistor model. Considering that metal films are more flexible, on the basis of a commonly adopted method for constructing the interface model [25]: the in-plane lattice constants of the transistor supercell is chosen as the same as those of the bulk ZnO. For simplicity, such treatment is applied by elongating the in-plane lattice constants of Ag(1 1 1) layers in order to eliminate the lattice mismatch between the two materials in our model. By using the treatment in previous theoretical study [22,23,25], the theoretical model is stable and has a simple structure. Therefore, the treatment simplifies the complexity of calculations. The structure of the Ag/ZnO interface is assumed as follows [25-28]: for ZnO(000$\bar{1}$)-Ag interface (Ag-O polar surface), Ag atoms tend to lie on the

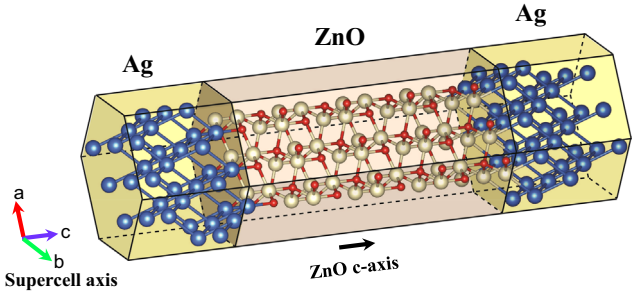

Fig. 1 Schematic illustration of a Ag-AnO-Ag piezotronic transistor and its atomic structure model, with the *c*-axis of ZnO is indicated.

Please cite this article as: W. Liu, et al., First principle simulations of piezotronic transistors, Nano Energy (2014), http://dx.doi.org/10.1016/j.nanoen.2014.10.014