



A theoretical study on the metal contacts of monolayer gallium nitride (GaN)

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ABSTRACT

Low-Schottky barrier height (SBH) metal contacts to 2D materials is indispensable for achieving high performance in atomic layer 2D materials channel based optoelectronic devices. In this study, we systematically investigate the detailed face contact properties of monolayer (ML) hexagonal gallium nitride (GaN) with six different commonly used metals (Au, Ag, Pd, Pt, Ti, and Ni) in field-effect transistors (FETs) utilizing the first principles electronic structure calculations based on density functional theory (DFT). It is found that no tunnelling barriers (TB) exist in all the ML GaN-metal face contact systems by calculating and analyzing the average effective potentials (V_{eff}). Moreover, ML GaN undergoes a vanishing of Schottky barriers in the vertical interfaces by analyzing the binding energy, electron localization function (ELF), and projected state density (PDOS) of six contact combinations. In terms of the energy band calculation, ML GaN forms n-type Schottky contacts with Au, Pd, Pt and Ti electrodes, and an n-type ohmic contacts with Ag electrode, while a p-type ohmic contact with Ni electrode is obtained in the lateral interfaces. The results would provide an insight into the ML GaN-metal interfaces, and be beneficial for developing low dimensional GaN-based devices with high performance.

1. Introduction

The other two-dimensional (2D) architectural materials “beyond graphene” have attracted extensive attention in the past two decades and possess potential applications in nano-electronics and optics due to their peculiar photoelectric properties [1–5]. Among these materials, layered hexagonal boron nitride (hBN), with its wide bandgap energy (5.0–6.0 eV), has clearly established that 2D nitrides are key to advanced novel devices [6,7], which has opened a new field of materials research with promising applications in nano-electronic devices such as field-effect transistor (FET), which inspires researchers to search for other possible 2D nitrides “beyond hBN” [8,9]. As a well-known III-V compound semiconductors, GaN plays an important role in the field of optoelectronic devices such as light-emitting diodes [10], solar cells [11] and photo-detectors [12]. GaN-based nanowires (1D) have already been identified as promising candidates for the next generation photoelectric devices [13]. Even though, theoretical and experimental research on 2D GaN is still deficient and is expected to open up a new avenue for the research of optoelectronic devices. 2D monolayer (ML) GaN has been investigated about its mechanical, electronical, and optical properties by using density-functional theory. And it also has been

proved that it can form stable, planar, single-layer honeycomb 2D crystalline structures at high temperature [14–17]. The bulk GaN is a direct-band-gap material, while ML GaN has a relatively wider indirect bandgap. Lots of theoretical researches have been concentrated on the electronic and magnetic properties of ML GaN combined with impurities by way of adsorption and incorporation [18–21]. The mechanical characteristics of ML GaN under uniaxial tension using classical molecular dynamics has been studied [22]. Experimentally, a ML GaN with honeycomb structure has been synthesized via a migration-enhanced encapsulated technique with the use of graphene and maintains its structural stability as recently reported by Balushi *et al.* [17]. Subsequently, theoretical calculations have investigated the physical properties of 2D GaN, as well as other III–V semiconductors [23,24]. Stability as recently reported, indicating that 2D GaN is prospective for applications in energy conversion [25]. In addition, it should be noted that the various applications of ML GaN in devices are closely related to their contacts with metals, which require a comprehensive study of interfacial properties of ML GaN contacting with metals. However, the existence of large contact resistance is the major challenge that masks the intrinsic exceptional electronic properties of 2D materials [26]. Metal-semiconductor contacts are often associated with a formation of a

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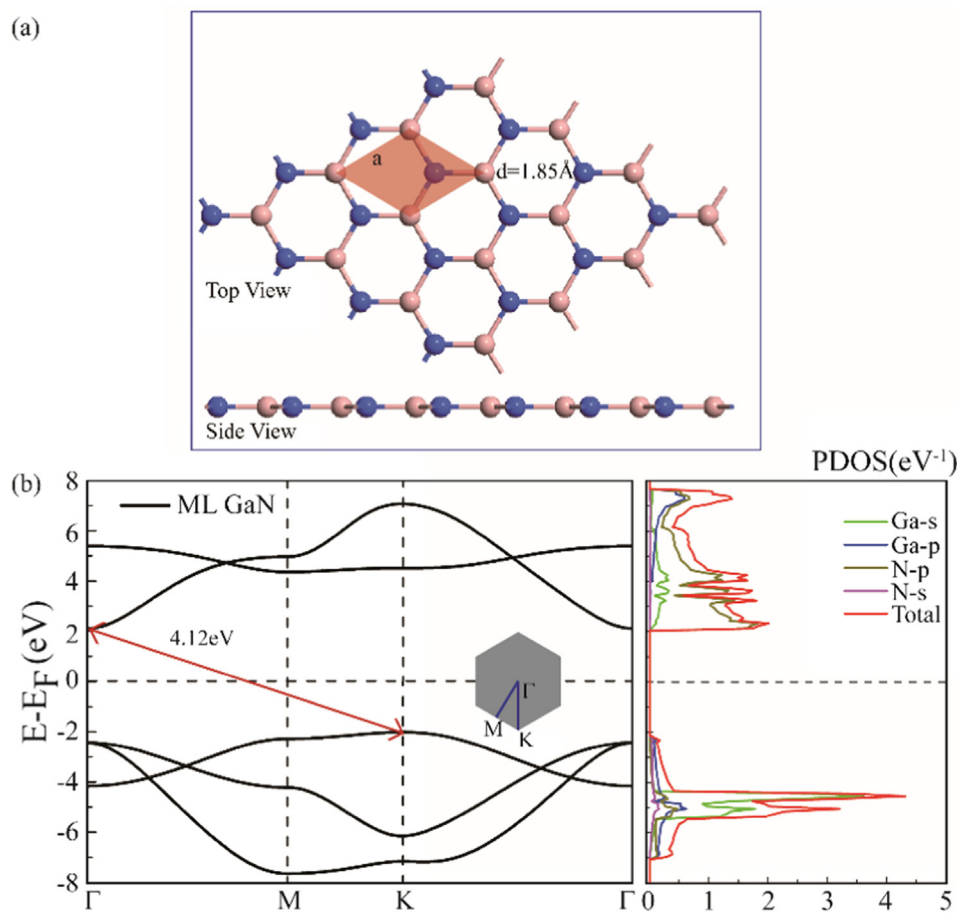


Fig. 1. (a) Top and side views of the optimized atomic structure of ML GaN. The 2D hexagonal primitive unit cell is delineated by rhomboid shadow area. The optimized lattice constant a and Ga–N bond length of d are indicated. The blue and purple balls denote Ga and N atoms, respectively. (b) Calculated electronic energy band structure of the optimized structure of ML GaN is presented along major symmetry directions of the Brillouin zone shown by the inset and the indirect band gap E_g is indicated. The Fermi level is set as zero energy (the dashed lines).

finite Schottky barrier height, which decreases the carrier injection efficiency. Apparently, decreasing Schottky barrier height (SBH) is critical to reach high performance devices, and a low resistance ohmic contact with vanishing SBH is highly desirable. The SBH does not only depend on the difference between the intrinsic Fermi level (E_F) of a metal and the CBM or VBM of the semiconductor but also is controlled by the interfacial nature of contact region according to previous research [27]. Besides, a good contact with metal is as crucial to the performance of the devices as the semiconductor itself due to a lack of controllable and sustainable substitutional doping way in 2D materials. Until now, the interfacial properties between ML GaN and Au, Ag, Pd, Pt, Ti and Ni 3D metal electrodes based on a periodical system have not been studied theoretically. Thus, a comprehensive understanding of the nature of the ML GaN-metal interface has become particularly important.

In this work, we investigate the electronic interfacial properties of monolayer freestanding ML GaN contacts with six different metals (Au, Ag, Pd, Pt, Ti, and Ni). We firstly calculate the binding energy (E_b) and the physical separation $d_{\text{GaN-M}}$ (M being the metallic atom) applying the first-principles calculations based on density functional (DFT). It is found that the interaction between ML GaN and Au, Ag surfaces is weaker than that of Pd, Pt, Ti, and Ni. Moreover, ML GaN undergoes a metallization on the six metal electrons in the vertical directions by analyzing the electron localization function (ELF) and the PDOS of six contact systems. In consideration of the lateral directions, ML GaN form Schottky contacts with Au, Pd, Pt, Ti (n type) metals, with lateral SBH of 1.35 eV, 0.37 eV, 1.22 eV, and 1.36 eV, respectively. And it forms an n type ohmic contact with Ag metal, while a p type ohmic contact with Ni metal is formed in terms of energy band analysis.

2. Methodology

The binding energy and different electronic properties for ML GaN-Metal interface geometries are characterized via the first-principles calculations with density-functional theory (DFT). All calculation were carried out with the Atomistic-ToolKit (ATK) version 2017.0 QuantumWise A/S (www.quantumwise.com) [28], which is based on the Kohn–Sham Density Functional Theory (KS-DFT) [29,30]. To take into account the exchange-correlation interaction of electrons, we chose the Perdew–Burke–Ernzerhof (PBE) functional [31] within the generalized gradient approximations (GGA). The van der Waals interactions between the 2D materials and metals are modeled using the DFT-D2 [32]. The density mesh cutoff is set as 100 Hartree. As is well known, the standard GGA methods often cannot calculate the bandgap accurately and the GGA1/2 method is able to correct the band error in both bulk and 2D materials [33]. Therefore, we adopt GGA1/2 method to correctly obtain the 4.12 eV bandgap of GaN, which is consistent with the previous theoretical results [17], as shown in Fig. 1(b). Besides, pseudopotentials of gallium (Ga) and nitride (N) are generated using the Hartwingster–Goedecker–Hutter [34] scheme with Tier 4 basis set. The iteration control parameters consist of Pulay mixer algorithm using 100 as a maximum number of iteration steps and the force is less than 0.01 eV/Å on each atom. The energy between two successive steps is less than 10^{-5} eV. During the relaxation, the Brillouin zone is sampled by $3 \times 3 \times 1$ Monkhorst–Pack k-point meshes. $16 \times 16 \times 1$ Monkhorst–Pack k-point meshes are used to calculate the partial densities of states (PDOS) [35]. The atomic structure of ML GaN in Fig. 1(a) shows the top view (upper panel) and side view (lower panel) of ML GaN honeycomb lattice. A supercell with a thick vacuum buffer region (15 Å) along the c-axis is employed, which ensures that the spurious interactions between the layers are negligible. The atomic

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