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Two dimensional hole gas induced by the heterointerface of nonpolar plane AlN(1 $\bar{1}$ 0 0)/H-terminated (1 0 0) diamond

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ABSTRACT

Tailoring the electronic states of the AlN/diamond (AlN/C) interface is critical to develop the next generation semiconductor devices such as the deep-ultraviolet light-emitting diode, photodetector, and high-power high-frequency field-effect transistor. In this work, we investigate the electronic properties of the nonpolar plane AlN(1 $\bar{1}$ 0 0)/H terminated (1 0 0) diamond heterointerface by using first-principles method with regard to different surface structures of diamond (1 0 0) plane, a semiconductor feature is predicted at the interface of nonpolar plane AlN(1 $\bar{1}$ 0 0)/C(1 0 0), and a two dimensional hole gas (2DHG) is generated when diamond surface is terminated by hydrogen. The charge transfer at the interface strongly depends on the surface termination of diamond, on which hydrogen suppresses the charge exchange at the interface. The band alignments of AlN/C heterostructures show a typical electronic character of the type-II staggered band configuration. The hydrogen-termination of diamond markedly increases the band offsets with a maximum valence band offset of 2.7 eV and a conduction band offset of 2.0 eV for the AlN(1 $\bar{1}$ 0 0)/C(1 0 0). The observation of the 2DHG at the nonpolar AlN(1 $\bar{1}$ 0 0)/HC(1 0 0) interface and the larger band offsets open the avenue for the development of novel high-power, high-frequency diamond power devices.

1. Introduction

Diamond (C) has attracted wide interest as an extreme semiconductor material for next generation power and photoelectronic devices owing to the wide-bandgap, the highest thermal conductivity, high breakdown field, high carrier mobility, and high carrier saturation velocity among all the available semiconductors [1]. The practical application of semiconductor diamond electronic devices relies on the reduction of the electrical resistivity of diamond by doping impurities and the control of the interface formed between diamond and other materials. Despite the lack of shallow dopants at this moment, the hydrogenated diamond surface exhibits a unique p-type surface conductivity with a hole density around 10^{13} cm^{-2}[2]. Such a surface conductivity has opened the avenue for the development of metal-semiconductor or metal-oxide semiconductor field-effect transistors (FETs), which showed exciting performance like high cut-off frequency and capability operating at high temperatures [3,4]. Another important structure is the hetero pn-junction, which is the basis for the development of deep-ultraviolet photoelectronic and power devices [5]. Among all these heterostructures, the interfaces properties at the junctions of diamond with other materials determine the ultimate device performances.

One promising junction is the AlN/C heterostructure, in which both AlN and diamond are wide-bandgap semiconductors. The AlN/C heterostructure is expected to lead to a variety of novel semiconductor devices such as deep-ultraviolet (DUV) light emitting diode, DUV photodetector, and high power FETs. Experimentally, the implementation of AlN/C pn-junction diode and field-effect transistors has already been demonstrated [6–8]. Although single crystal AlN epitaxial layer on diamond could be achieved, the existence of a large amount of interface states is anticipated due to the large lattice mismatch between the hexagonal AlN and the cubic diamond. The high concentration defects degrade the devices performance such as the appearance of sub-bandgap emission and the low efficiency of band-to-band recombination in pn-junction diodes and high leakage current in electronic devices. Therefore, the understanding of the interface character of the AlN/C heterojunction is in demand for the development of the next generation optoelectronic devices operating at DUV region and electronic devices for high power and high frequency applications.

However, few experimental values [7] or theoretical results [9,10] are available on the interface characteristic parameters of

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the AlN/C heterostructure. The reported calculations are focused on polar plane AlN(0 0 0 1)/C(1 0 0) heterointerface, where the average valence-band offset, a staggered (type II) band alignment and the presence of a large number of interface states in the band gap were predicted[9,10]. The interfacial electronic properties are good agreement with our computational results at the polar plane AlN(0 0 0 1)/C(1 0 0) and the semipolar plane AlN(1 $\bar{1}$ 0 1)/C(1 0 0) heterointerface, which are not presented here. The different electronic properties at the nonpolar plane AlN(1 $\bar{1}$0 0)/C(1 0 0) heterointerface are only shown in this work.

For chemical vapor deposition (CVD) single crystal diamond, the most important crystallographic surface of is the (1 0 0) surface, on which most of the homoepitaxial growths and devices fabrication have been performed. Due to the existence of dangling bonds, the (1 0 0) surface appears with a 2×1–(1 0 0) surface reconstructions for the clean surface (C(1 0 0)) and 2×1–(1 0 0):H reconstruction for the surface with hydrogen termination (HC(1 0 0)) [11–14]. Another feature of H-diamond is the negative electron affinity [15], which allows the formation of a high interface barrier for diamond heterojunction devices and facile electron emitting source. First in this paper, different diamond surfaces such as the clean reconstructed 2×1–(1 0 0) surface (C(1 0 0)) and H-terminated diamond 2×1–(1 0 0) surface (HC(1 0 0)) are examined. Then the interfacial characteristics of the nonpolar plane AlN(1 $\bar{1}$ 0 0)/C(1 0 0) heterointerface are theoretically calculated and analyzed.

2. Computational and modeling details

2.1. Methods

The total-energy and physical properties calculations were carried out with Vienna *ab initio* Simulation Package (VASP) based on density-functional theory (DFT) within the generalized gradient approximation (GGA) [16–18]. The projector-augmented wave pseudo-potentials and the exchange correlation functional of Perdew, Burke, and Ernzerhof for the GGA were utilized in the simulation [19]. Valence electron configurations for the elements were $2s^2 2p^2$ for C, $3s^2 3p^1$ for Al and $2s^2 2p^3$ for N. The Monkhorst–Pack scheme was employed for the Brillouin zone integration with a $5 \times 9 \times 1$ k-point mesh. In the energy minimization, we constrain the lattice constant of AlN/C hetero-structure to the average value

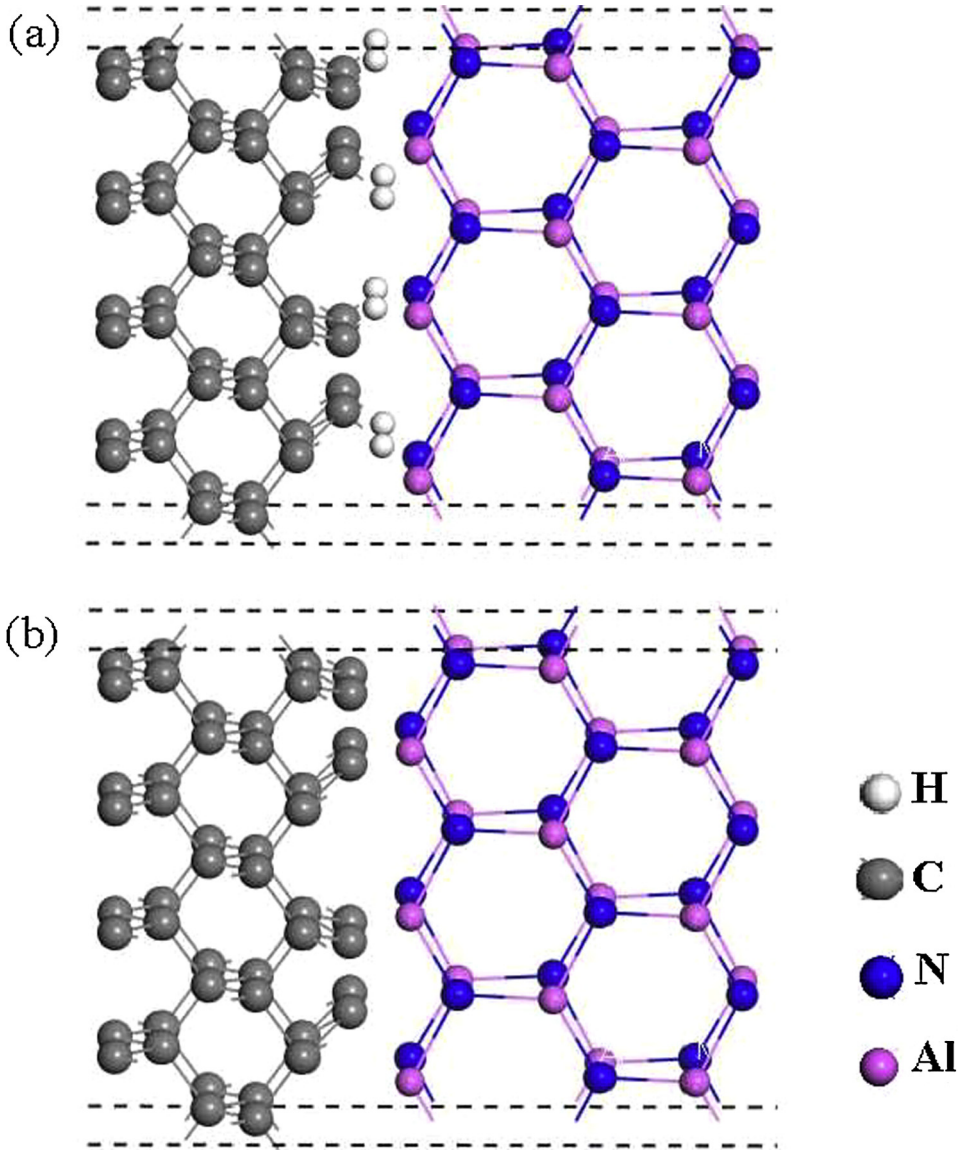

Fig. 1. Slab models of nonpolar plane AlN(1 $\bar{1}$ 0 0)/C(1 0 0) interface (a) with and (b) without H.