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Calculation of Electronic Structure Properties Of Two-Dimensional AlN/SiC Heterojunction Under Biaxial Stress

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ABSTRACT

Under the action of in-plane biaxial stress, the electronic structure properties of the two-dimensional AlN/SiC heterostructure were studied by first principles. The two-dimensional AlN/SiC heterostructure has an indirect band gap in its original state, and the band gap can be adjusted under -10%~10% biaxial strain, without the transition to direct band gap and metal. The application of in-plane biaxial stress can effectively adjust the electronic characteristics. Based on the calculation of the energy band, the influence of the external biaxial tensile strain on the effective carrier mass is discussed. The results show that the band gap of the two-dimensional semiconductor material can be adjusted by the in-plane biaxial strain. It has the expected application value.

KEYWORDS

AlN / SiC heterostructure; Biaxial stress; Electronic structure characteristic; Effective mass

1. INTRODUCTION

Since the successful exfoliation of graphene from graphite in 2004, it has shown broad application prospects in electronics, aerospace, and everyday life due to its unique physical properties. In recent years, researchers around the world have been competing to discover new two-dimensional (2D) materials, such as transition metal dichalcogenides(TMDs) [1][2], borophene [3-4], black phosphorus, blue phosphorus [5-6], and other 2D carbides and nitrides [7-9]. These 2D materials possess exceptional electronic and optical properties different from bulk materials and hold potential for applications in next-generation nanoscale semiconductor devices, chemical catalysts, solar cell materials, and energy storage materials [10-12].

Aluminum nitride (AlN) is a III-V cluster semiconductor recognized for its outstanding thermal conductivity, good piezoelectric performance, high resistance, and low thermal expansion coefficient at high temperatures [13-14], making it an extremely attractive material. Compared to compound semiconductors like sapphire and SiC, AlN crystals have similar lattice constants and thermal expansion coefficients to materials such as GaN and AlGaN [15], and possess a wider bandgap [16]. Unlike borophene or boron nitride (BN) materials, single-atom-layer AlN has not yet been synthesized; only a few experiments have reported the epitaxial growth of AlN monolayers on various crystalline substrates such as Si and Ag [17-18]. Experiments using electron diffraction and scanning tunneling microscopy on metallic Ag have confirmed that AlN has a graphite-like hexagonal structure and a larger lattice constant compared to bulk wurtzite AlN. Fortunately, theoretical calculations provide another method for studying the physical properties of AlN. First-principle calculations indicate that the hexagonal single-layer AlN, with an indirect bandgap of 2.91eV (GGA) and 1.81 eV (GW), is a dynamically stable structure [19]. Notably, theoretical predictions suggest potential applications of monolayer AlN as a photocatalyst [20-21]. Bulk silicon carbide (SiC), like AlN, is widely used in micro-electrochemical systems and in high-temperature, high-frequency, and high-

power electronic devices, offering advantages such as a wide bandgap, high strength, high saturated carrier mobility, and high thermal conductivity. Single-layer SiC has not yet been synthesized experimentally recently; however, Lin managed to produce ultra-thin SiC nanosheets with thicknesses ranging from 0.5 - 1.5 nm in solution through mechanical exfoliation [22], which structurally resembles graphene. Although the two-dimensional honeycomb structure of SiC monolayer has not been synthesized yet, calculations based on density functional theory (DFT) indicate that single-layer SiC is a stable semiconductor material, with a bandgap of 2.53eV under GGA approximation and 3.90 eV under GW0 correction [23]. Additionally, SiC nanosheets have been reported in the literature as a promising photocatalytic material with many excellent physical properties.

Constructing van der Waals heterostructures is a method to discover and enrich material physics phenomena, especially prominent in enhancing carrier mobility and visible light absorption, playing a crucial role in modern electronic and optoelectronic devices. Given the matching hexagonal crystal structures of AlN and single-layer SiC [18-23], building an AlN/SiC van der Waals heterostructure is a worthwhile bimolecular layer to explore. This paper first utilizes first-principle calculations based on DFT to study the electronic and photocatalytic properties of the AlN/SiC vdW heterostructure, and then analyzes the effects of an external electric field and in-plane biaxial strain on the electronic and photocatalytic properties of the AlN/SiC heterostructure. Our goal is to provide a theoretical foundation for the research on AlN/SiC vdW heterostructures, with broad application prospects in future nanodevices and solar cell materials.

2. COMPUTATIONAL METHODS

This article utilizes the Vienna Ab-initio Simulation Package (VASP) for simulating the AlN/SiC heterostructure. Interactions between atoms are described using the Projector Augmented Wave (PAW) method based on density functional theory (DFT). Electron correlation interactions are modeled using the Generalized Gradient Approximation (GGA) with the Perdew Burke Ernzerhof (PBE) exchange-correlation potential. The plane-wave cutoff energy is set to 500 eV, and the valence electron wave functions are expanded using Gaussian smearing with a broadening width of 0.03 eV. Given the lattice mismatch of less than 5% between AlN and SiC, the heterostructure is constructed by stacking 1x1 monolayers of AlN and SiC in the z-direction perpendicular to the interface. A 2 nm vacuum layer is added in the z-direction to prevent non-local exchange interactions between the layers of the AlN/SiC van der Waals heterostructure. Brillouin zone sampling is performed using the Monkhorst-Pack method centered at the Γ point, with a k-point grid of 9x9x1. Structural optimizations are carried out using the GGA conjugate gradient method, with electronic self-consistent iteration convergence criteria set at 1.0x10^-5 eV/unit and ionic relaxation convergence criteria requiring forces on each atom to be less than 0.01 eV/Å. To accurately account for van der Waals forces, the DFT-D3 method proposed by Grimme is employed. Additionally, bandgap variations for several systems are determined using the Heyd-Scuseria-Ernzerhof hybrid functional (HSE06). Specifically, both HSE06 and PBE calculations are conducted on the AlN/SiC heterolayer as a unique system.

Currently, there are two effective methods for altering the electronic structure properties of two-dimensional materials: applying an external electric field and in-plane stress. In this paper, we primarily investigate the effect of in-plane biaxial stress on the electronic structure properties of the two-dimensional AlN/SiC heterostructure.Biaxial stress is applied to the AlN/SiC heterostructure by simultaneously altering the lattice parameters in both the a and b directions.The calculation for biaxial tensile strain (ε) is as follows:

$$\varepsilon = (a - a_0) / a_0 \times 100\% \quad (1)$$

Here, α represents the lattice parameter of the crystal under applied strain, and α0 is the lattice parameter of the crystal in its equilibrium state without strain. The applied strain ranges from −10% to +10%, where "+" indicates tensile strain and "−" indicates compressive strain. After structural optimization under the given strain conditions, the band structure and photocatalytic properties are calculated and analyzed.

In addition to having an appropriate bandgap, higher carrier mobility is also a crucial factor for semiconductor materials used in nanoelectronic devices. The primary factor determining carrier mobility is the effective mass of the carriers. The effective mass of carriers is material-dependent, and electrons and holes have different effective masses in various semiconductors. To gain a deeper understanding of the electronic structure properties of two-dimensional heterostructures, we investigated their effective electron and hole masses.The effective masses of electrons and holes can be obtained by fitting a parabolic function to the energy bands near the valence band maximum (VBM) and conduction band minimum (CBM) of the AlN/SiC heterostructure:

$$m^* = \pm h^2 \frac{d^2 E_k}{dk^2} \tag{2}$$

h is the reduced Planck constant, k is the wave vector, E_k is the energy corresponding to the wave vector k.

3. RESULTS AND DISCUSSION

3.1. Geometric Structure

We constructed a two-dimensional AlN/SiC van der Waals heterojunction, where the atoms are positioned in an x-y plane with periodic boundary conditions, and a 20 Å vacuum is applied along the z-axis to eliminate interactions between adjacent layers. The heterojunction is composed of two graphene-like materials, which can be stacked in various configurations, described as PI-type, PII-type, and PIII-type, depending on how a single layer of AlN is stacked on top of a single layer of SiC. We selected three relatively stable configurations for calculating their binding energies, from which we chose the most stable one for further study of its electronic structure properties. The three relatively stable configurations are shown in Figure 1.

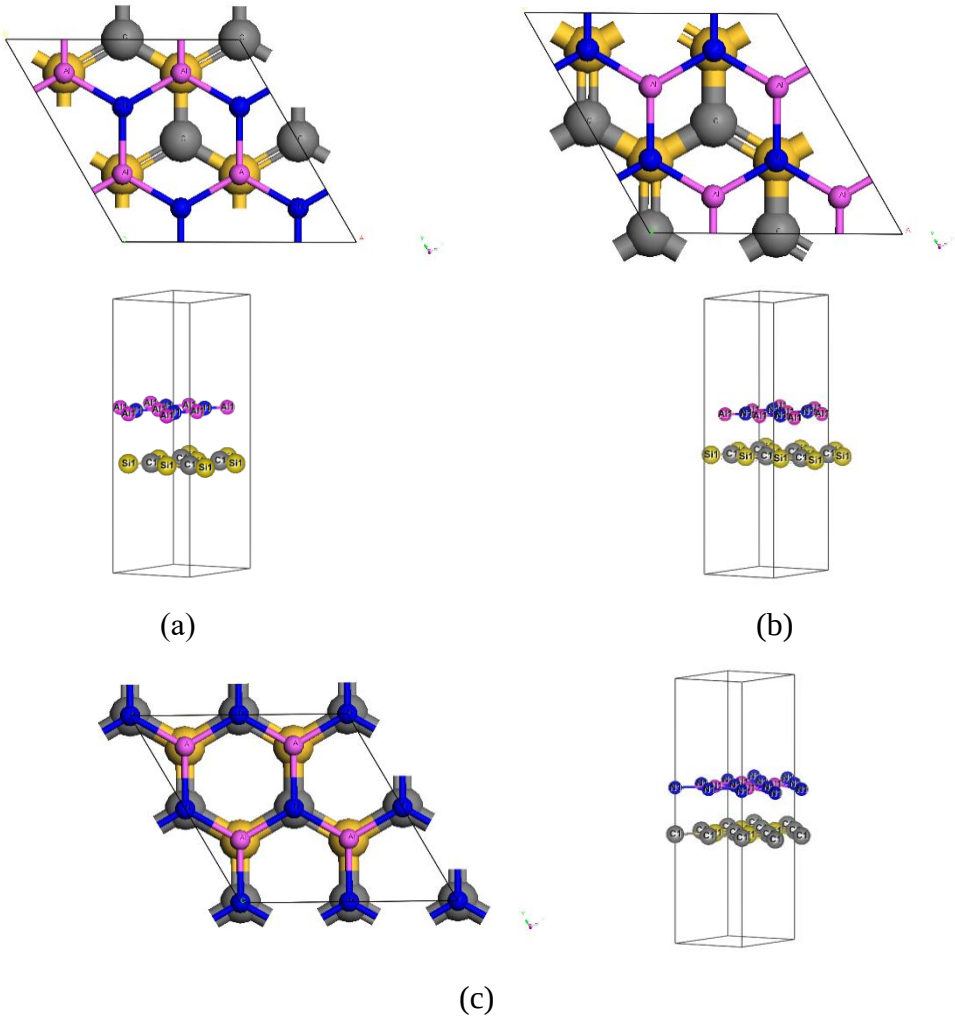

Figure 1. Two-dimensional heterojunction AlN/SiC different stacking methods: (a) is PI, (b) is PII, (c) is PIII. In the picture, the yellow balls represent Si atoms, the gray balls represent C atoms, the blue balls represent N atoms, and the pink balls represent Al atoms.

The lattice parameters and Si-C (Al-N) bond lengths of SiC (AlN) crystals were optimized using the PBE exchange-correlation functional. The optimized values are 0.310 nm (0.314 nm) and 0.179 nm (0.182 nm), respectively, which are consistent with other reported computational results (0.307 nm (0.312 nm) and 0.177 nm (0.180 nm)) [19] and experimental values (0.310 nm and 0.179 nm) [20].

Lattice matching is crucial for heterostructures, and the lattice mismatch between monolayer AlN and SiC is less than 1.0%, meeting the ideal conditions for preparing vdW heterostructures. Therefore, we designed three different stacking configurations, described as PI, PII, and PIII, as shown in Figure 1. Each AlN/SiC heterostructure model can be transformed into another by horizontally sliding the single atomic layer. As we know, the binding energy (E_b) can be used to evaluate the structural stability of heterostructure systems and is defined as:

$$E_b = E_{AlN/SiC} - E_{AlN} - E_{SiC} \tag{3}$$

In this formula, $E_{AlN/SiC}$ is the total energy of the AlN/SiC vdW heterostructure, E_{AlN} is the total energy of the independent monolayer AlN, and E_{SiC} is the total energy of the independent monolayer SiC. The total energy (E_{tot}), interlayer distance (d_{int}), and binding energy (E_b) for the three stacking configurations are listed in Table 1. The binding energy E_b is defined such that a negative value indicates an exothermic (stable) adsorption process, while a positive value indicates an endothermic (unstable) adsorption process. The E_b values for the AlN/SiC heterostructures are all negative, indicating stable binding of the heterostructures. It is well known that the more negative the formation

energy, the more stable the structure, and the larger the absolute value of the binding energy, the more stable the heterostructure system. As shown in Table 1, the PII-type stacking configuration has a formation energy of −4.706 eV/unit, making it the most stable among the three. The calculated interlayer distance (0.3751 nm) is much greater than the sum of the covalent radii of N and Si atoms, indicating that their interaction is within the van der Waals force range. This confirms that AlN and SiC form a stable van der Waals heterojunction. Below, unless otherwise stated, we will focus on the PII-type structure to study its strain effects.

Table 1. Interplanar spacing d, total energy E_{tot}, binding energy E_b corresponding to three different stacking methods, * indicates the most stable stacking method for two-dimensional heterojunction AlN/SiC

Stacking Configuration	d_{int} (nm)	E_{tot} (eV)	E_b (eV)
PI	0.4052	-25.804	-1.409
PII (*)	0.3751	-29.101	-4.706
PIII	0.4216	-29.059	-4.654

3.2. Electronic Structure Properties

The band structure and electronic density of states (DOS) are two important physical quantities for studying the electronic properties of materials. We calculated the DOS, band structure, partial density of states (PDOS), and projected band structure of the heterojunction. These quantities clearly demonstrate the electronic coupling and orbital contributions between the components. Figures 2(a), 2(b), and 2(c) show the band structures and projected band structures of 2D monolayer AlN, SiC, and the AlN/SiC heterojunction, respectively. The red lines in the band structure are the results obtained using density functional theory (DFT) with the PBE pseudopotential, while the blue lines are obtained using DFT combined with the HSE hybrid potential.

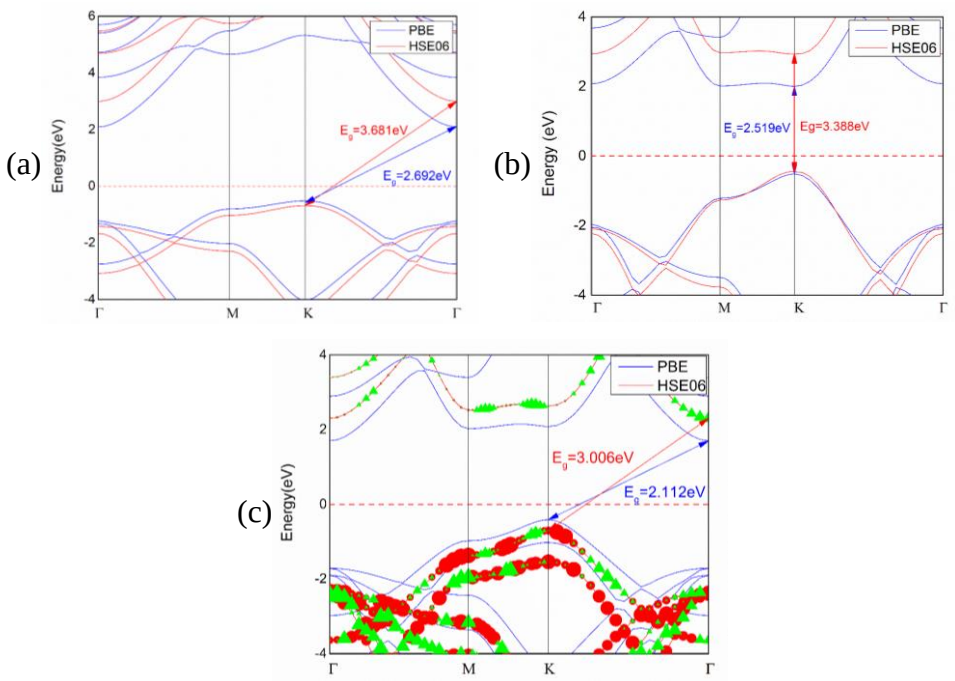

Figure 2. (a) Single-layer AlN energy band diagram. (b) Single-layer SiC energy band diagram. (c) Energy band diagram of two-dimensional AlN/SiC heterojunction. Blue indicates PBE method, red indicates hybridization in the functional HSE06 method, the red point represents the projection energy band of AlN, and the green triangle represents the projection energy band of SiC.

In Figure 2(c), the red and green circles on the AlN and SiC bands represent the contributions of AlN and SiC bands in the heterojunction. From Figures 2(a) and 2(b), it is evident that monolayer AlN is

an indirect semiconductor with a bandgap of 3.681 eV (HSE06), where the conduction band minimum (CBM) and valence band maximum (VBM) are located at the high-symmetry Γ and K points, respectively. Monolayer SiC is a direct semiconductor with a bandgap of 3.388 eV (HSE06), with both the CBM and VBM located at the K point.

From Figure 2(c), we can see that the AlN/SiC heterojunction is an indirect bandgap semiconductor with a bandgap of 3.006 eV (HSE06) and 2.112 eV (PBE). It is well-known that the PBE method can produce the correct bandgap shape but tends to underestimate the bandgap. The CBM is at the Γ point, while the VBM is at the K point. Results verified using the more precise HSE06 functional show a similar band structure but with a wider indirect bandgap of 3.006 eV (Figure 2c).More importantly, compared to monolayer AlN and SiC, the AlN/SiC heterostructure has a suitable bandgap for use as a photocatalyst.

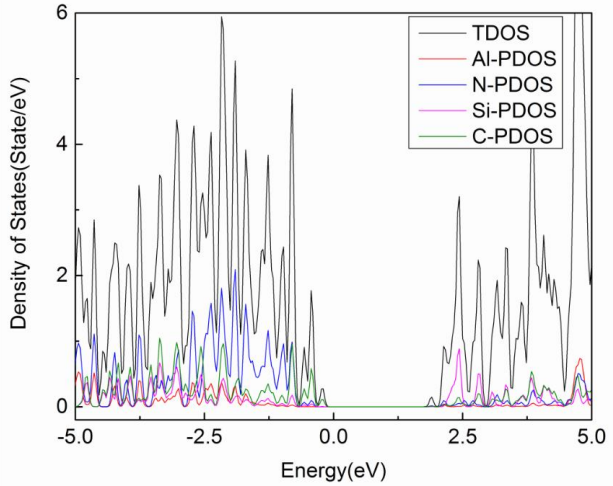

Figure 3. Total density of states of two-dimensional AlN/SiC heterojunction and partial density of states of Al, N, Si and C atoms

To further explore the electronic properties of the AlN/SiC heterostructure, Figure 3 shows the total density of states (DOS) and the projected density of states (PDOS). It can be seen that C atoms contribute to the VBM, while N and Si atoms contribute to the CBM of the heterostructure. Thus, the formation of AlN/SiC, through van der Waals interactions, results in a band alignment that forms an indirect bandgap type-II heterojunction. This type of heterojunction is beneficial for the effective separation of photoexcited electrons and holes.

3.3. Effects of Applied Strain

It has been demonstrated that applying external strain is a powerful tool for altering the electronic properties of two-dimensional materials [6-27]. Previous studies have reported that silicon carbide has considerable stability, with uniaxial and biaxial tensile strains reaching up to 10% [28-29], indicating that the AlN/SiC heterojunction exhibits good strain tolerance. Figure 4 shows the band structures corresponding to strain ranging from -10% to 10%, with a strain interval of 4%. From the band structure, we can see that 2D AlN/SiC remains an indirect semiconductor, with the valence band maximum (VBM) located at the high-symmetry K point and the conduction band minimum (CBM) at the high-symmetry Γ point in the Brillouin zone. This characteristic does not change with compressive or tensile stress, reflecting the excellent compressive resistance and stability of the 2D AlN/SiC heterojunction.

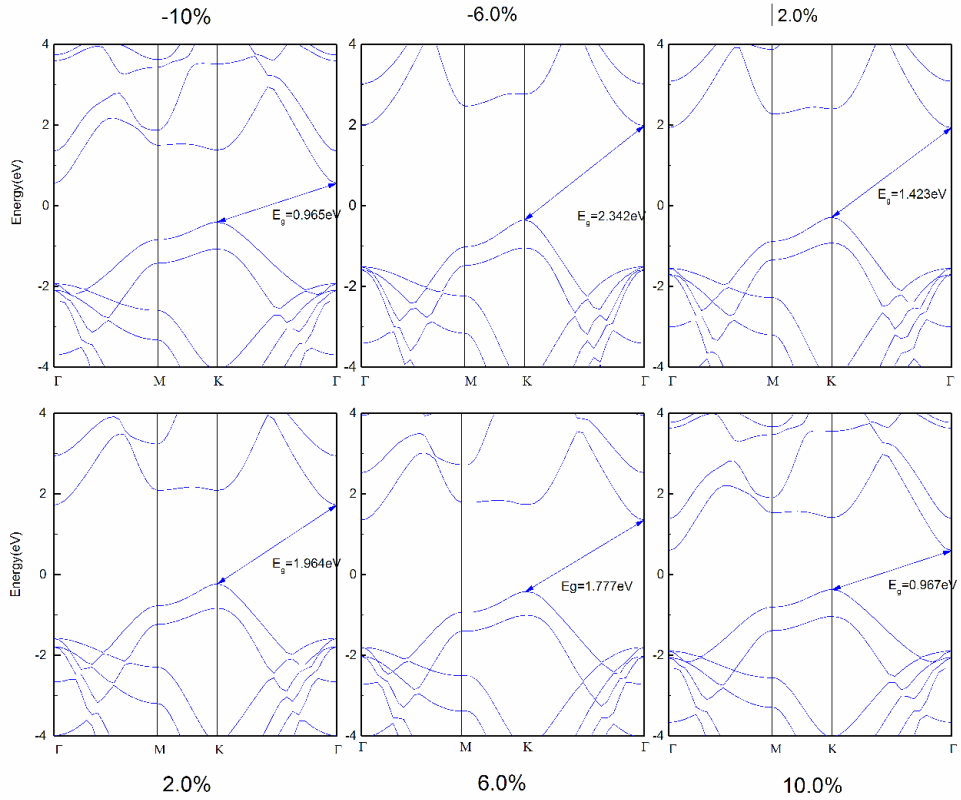

Figure 4. Two-dimensional AlN/SiC band diagram under different strains

As the tensile strain increases, the CBM shifts downward toward the Fermi level from 0% to 10%, while with increasing compressive strain, it shifts upward away from the Fermi level from 0% to 10%, and the VBM shows almost no movement. Therefore, biaxial tensile strain plays an important role in modulating the bandgap of the AlN/SiC heterojunction, indicating its promising application prospects in strain sensors.

To gain a deeper understanding of the electronic properties of the AlN/SiC heterojunction, we investigated the effective masses of electrons and holes near the VBM and CBM under biaxial tensile strain, as shown in Table 2. In the table, "e" and "h" represent "electrons" and "holes," respectively. The high-symmetry k-point paths corresponding to the effective masses are indicated as subscripts.

As clearly shown in Table 2, the effective masses of electrons and holes along the Γ-K and Γ-M directions decrease with increasing tensile stress and increase with increasing compressive stress. The trend for the effective mass of electrons along the K-Γ and K-M directions is consistent with that along the Γ-K and Γ-M directions, whereas the trend for the effective mass of holes along K-Γ and K-M differs from that along Γ-K and Γ-M.

Table 2. Effective masses of electrons and holes near the bottom of the conduction band and the top of the valence band in AlN/SiC heterojunctions under different stresses

Stress (%)		-7	-5	-3	-1	0	1	3	5	7
e	$m^*_{\Gamma-M(\Gamma-K)}/m_0$	0.746	0.696	0.638	0.579	0.549	0.519	0.436	0.406	0.350
h	$m^*_{\Gamma-M(\Gamma-K)}/m_0$	-3.008	-2.854	-2.735	-2.632	-2.592	-2.552	-2.329	-2.434	-2.391
e	$m^*_{K-\Gamma}/m_0$	0.993	0.860	0.771	0.706	0.681	0.659	0.623	0.595	0.574
h	$m^*_{K-\Gamma}/m_0$	-0.546	-0.547	-0.550	-0.554	-0.557	-0.560	-0.567	-0.575	-0.584
e	m^*_{K-M}/m_0	1.410	1.146	0.985	0.878	0.837	0.802	0.746	0.705	0.673
h	m^*_{K-M}/m_0	-0.588	-0.589	-0.593	-0.597	-0.600	-0.603	-0.610	-0.619	-0.627

We know that, when considering only the effect of the periodic lattice, a smaller effective mass of carriers corresponds to higher carrier mobility. Therefore, tensile strain favors improving the carrier mobility of the AlN/SiC heterojunction. Moreover, under biaxial tensile stress, the effective mass of holes along the Γ-K and Γ-M directions is greater than that of electrons, while along the K-Γ and K-M directions, the effective mass of holes is smaller than that of electrons, indicating slightly higher electron mobility.

These results suggest that the AlN/SiC heterojunction holds great potential for applications in electronic and strain devices.

4. CONCLUSION

In summary, we investigated the electronic structure properties of the AlN/SiC heterojunction under biaxial tensile strain using first-principles calculations based on DFT-D2. Our calculations show that monolayers of AlN and SiC are bonded together through van der Waals interactions to form an indirect bandgap type-II heterojunction, which facilitates two types of redox reactions across different layers. In addition, we found that the application of biaxial tensile strain has a significant impact on the bandgap modification. We also calculated the band edges and the effective masses of electrons and holes under biaxial tensile strain. These results indicate that the AlN/SiC heterostructure is a novel 2D type-II indirect semiconductor, making it a promising material for fabricating optoelectronic devices.

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