



Structural stability and electronic properties of the (0 0 0 1) inversion domain boundary in III-nitrides

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ABSTRACT

A structural investigation of (0 0 0 1) plane inversion domain boundaries (IDBs) in group III-nitrides (GaN, AlN and InN) has been carried out by means of Monte Carlo (MC) simulation of Stillinger-Weber empirical potential. Eight possible IDB configurations were found to be stable during the structural searching process. Their energetics, chemical bonding properties as well as electronic structures were further investigated using first-principle calculations based on density functional theory (DFT). The comparison of relative energetic stability revealed that the H4 configuration is the most stable structure among H (Head-to-Head type) IDBs except in AlN; as for T (Tail-to-Tail type) IDBs, T2 is more energetic favorable within all materials. The electron localization function (ELF) and the Bader population analysis clearly point out 2-dimensional hole gas (2DHG) in H IDBs and 2-dimensional electron gas (2DEG) in T IDBs. And this is ascribed to the polarization discontinuity. A detailed analysis of Projected Density of States (PDOS) shows a metallic character in all IDBs. The hybridization states at the valance band edge crossed the Fermi level in H boundaries which acts as a p dopant. For T type IDBs, the PDOS is largely extended in density with the Fermi level shifted up above the conduction band maximum (CBM) which suggests an electron excess in boundaries.

1. Introduction

The Group III-nitrides (AlN, GaN and InN) have been considered as the promising materials in a wide range of applications from micro-electronics [1], optoelectronics [2] as well as high-temperature and high-power electronics [3] owing to their outstanding properties including direct band gap, high mechanical, thermal stability, large piezoelectric constants and so on [4,5]. Particularly, the use of heterostructures including their alloy system make them ideal materials for applications, such as InN/GaN- or AlN/GaN-based diodes [6] and AlGaIn/GaN- or InAlN-based high electron mobility transistors (HEMTs) [7]. Nevertheless, a large number of extended defects may be present inside the layers upon the growth of the heterostructures due to the lattice mismatch [8,9]. This critically effects the quantum efficiencies and device lifetime. Therefore, it is still essential to determine whether and how defects modify physical and the electronic properties in these materials.

Inversion domain boundary (IDB) is one of the archetypical planar defects which may form in noncentrosymmetric crystals. A large number of investigations have been reported on it since the concept of polarity inversion was first advanced by Aminoff and Broom in wurtzite

crystal [10]. Along the [0 0 0 1] growth direction, IDB in wurtzite structure commonly takes place at {1 0 $\bar{1}$ 0} prismatic plane. Depending on the topology analysis [9–14], eight possible configurations of {1 0 $\bar{1}$ 0} IDBs have been discovered, as reviewed by Kioseoglou [11,12], and their electronic properties are predicted. Meanwhile, plenty of experimental efforts have also made by using high resolution TEM to investigate their native structure and growth behavior [15–19]. Moreover, a transition from low-energy and electronically nonactive IDB* type to the high-energy and electronically active Holt-type one is found under the influence of stacking fault [20] with GaN.

In this hexagonal symmetry, the other type of IDB which is located in the (0 0 0 1) plane is the simplest type of crystallographic boundary that may be studied. However, up to now, only Kim and Goo reported a TEM observation of (0 0 0 1) plane IDB in ZnO material and proposed eight possible geometric models [19]. They concluded that the H3 type IDB could be the most stable structure in their sample by matching the high-resolution TEM images with the simulation images of geometrical models.

In the following, we report on our systematic investigation of the energetic stability, local physical and electronic properties of these eight possible IDB configurations as suggested by Kim and Goo. We

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discuss the relative structural stability, the changes in electron localization function (ELF), the Bader charge, as well as the electronic structure of all these inversion boundaries.

2. Methodology

The eight geometrical IDB configurations proposed by Kim and Goo [19] are investigated in AlN, GaN and InN compounds. As a starting point, we tested their stability using Monte Carlo (MC) simulation [21] with our modified SW parameters [22–24]. The MC simulation is performed in the following manner: an atom S_i is randomly chosen in system; and then its positions r_i are rescaled by a perturbation Δr without changing the atomic type. The rejection or acceptance of this attempt is examined using the energy difference of system with and without this displacement [25]. Subsequently, first-principle calculations with the slab geometry scheme is implemented using Vienna *ab initio* simulation package (VASP) [26,27] to calculate the total energies, charge transfer characters as well as the electronic properties. The slabs with stacking sequence of (AaBb)₉A-(Metal-polar) and (AbBa)₉A-(N-polar) are first constructed as substrates along [0 0 0 1] direction; The corresponding polarity inversed slabs starting with nitrogen atoms are put on the front metal surfaces with displacement of 1/3[1 0 $\bar{1}$ 0] to form H and T IDBs. Figs. 1 and 2 give the detailed interface configurations. The surfaces are saturated with virtual hydrogen (H*) which host corresponding fractional electron located straight along [0 0 0 1] direction for termination. A vacuum layer of ~ 24.434 Å thickness is set to avoid the artificial interactions and strain. In the supercells the in-plane coordinates (x and y directions) of atoms apart from boundaries are fixed. The relaxation along c-axis did not give rise to any significant change in the test calculations [28]. The exchange correlation functional adopts the generalized gradient approximation [29,30] with the U corrections (GGA + U) according to the approach of Ref. [31] and the pseudopotential uses the projector augmented-wave method (PAW) method [32]. The $21 \times 21 \times 1$ Monkhorst-Pack Gamma k-point mesh is applied for Brillouin zone sampling. The atomic positions are optimized until the force on each atom is less than 10^{-2} eV/Å, and the energy difference between two electronic steps reaches 10^{-6} eV. The valence electron configurations are chosen as: Al($3s^2 3p^1$), Ga

($3d^{10} 4s^2 4p^1$), In($4d^{10} 5s^2 5p^1$) and N($2s^2 2p^3$), respectively.

3. Results and discussion

3.1. Energetics

After being relaxed in MC simulation of SW empirical potential with a series of temperature test, we found that, those eight IDB configurations proposed by Kim and Goo remain stable for the III-nitrides at relative lower temperature (below 300 K) condition, and no new structures are obtained. IDBs are destroyed with high temperature due to the absence of symmetry. The calculated relative energies obtained by total energy calculation of DFT are utilized to make statement for the relative stability among those candidates, seen in Table 1. The number of atoms and polarity arrangements are different between H and T IDBs but are identical in H and T supercells respectively, therefore the relative energies are evaluated by taking total energy of H1 and T1 supercell as their respective reference. For H IDBs, H4 is the most stable one in GaN and InN materials with the energies slightly lower than those of H1 (~ 1 and 4 meV lower in GaN and InN respectively). This is understandable when comparing the atomic stacking sequences of H1 (A/B/A/C/B) and H4 (A/B/A/C/A) (seen in Fig. 1(a) and (d)). It can be seen that the first-nearest neighbors of interfacial cations are similar. The changes of stacking sequence take place at the second-nearest neighbors suggesting a small influence on energetics as reported by Yan and Al-Jassim [33] for IDBs in ZnO. Moreover, as compared with H1 IDB which hosts two violations of stacking rule, H4 possesses only one stacking violation which is expected to be more energetically favorable [34,35]. H2 and H3 IDBs have linear metal-nonmetal-metal bonding at boundaries and their calculated total energies are 46 and 650 meV higher than those of H4 in GaN and InN. As for AlN, H1/H4 have higher energies than H2/H3, which is at variance to the conclusion in GaN and InN. Bond length distribution analysis reveals that, in interface region, H1/H4 IDBs shows a deformation of $\sim 9.3\%$ in AlN, which is around 1.3% larger than those in GaN and InN. However, the bond length deformations of H2/H3 IDBs in AlN are rather small, 1.1% on average, when compare with the other two compounds. This may lead to a lower energy in H2/H3 with respect to H1/H4 in AlN.

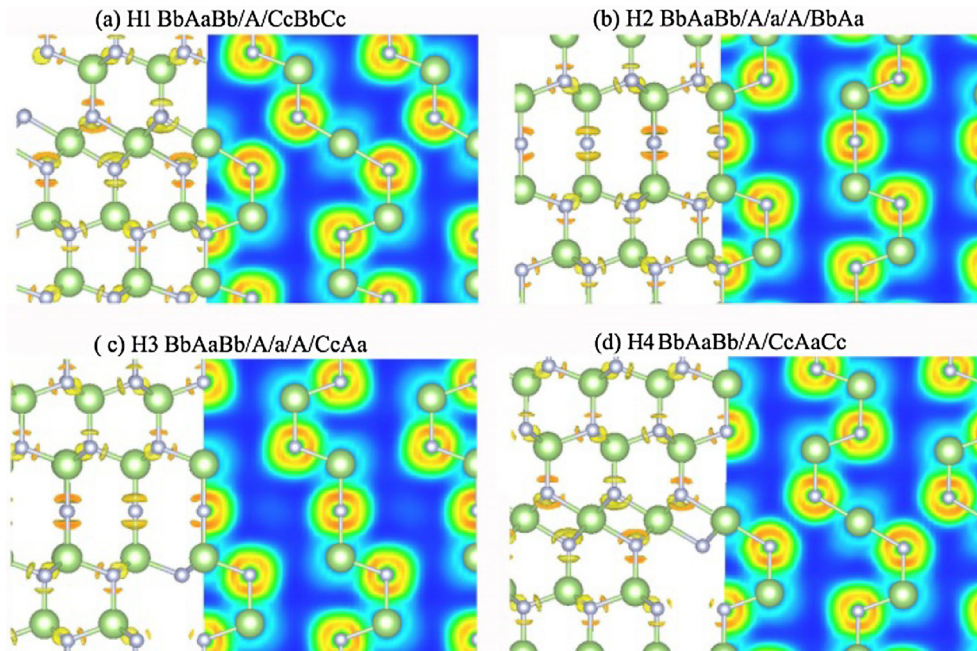


Fig. 1. ELF isosurface contours with $\eta = 0.823$ on the left-hand panel and the corresponding 2D contour slice crossing atomic plane on right-hand panel for H IDBs in GaN. The green and grey ball represent Ga and N atom, respectively. The respective atomic stacking sequences are shown on top: (a) H1, (b) H2, (c) H3 and (d) H4.

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