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Molecular-dynamics study of inversion domain boundary in w-GaN

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Abstract

The structures and the formation energy of inversion domain boundaries (IDBs) are investigated using the Tersoff empirical potential. Four kinds of IDBs (A and B types for IDB* and Holt) are considered. The IDBs with A type are energetically favorable compared to B type with the structural instability. The IDB* is also more stable than the Holt type in spite of fourfold and eightfold rings of bonds. We calculate the atomic configurations of the Holt IDBs induced by the interactions of the IDB* with the stacking faults I_1 and I_2. The stacking fault I_2 interacted with I_1 on the IDB induces the structural transformation from IDB* to Holt type. In the growth simulation of GaN on GaN surface with the IDB* type, the IDB* is shown in spite of its structural distortion.

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Keywords: GaN; Molecular dynamics; Inversion domain boundary

1. Introduction

GaN is a promising semiconductor material that exhibit many outstanding physical and chemical properties in high-temperature optoelectronics and high-power, high-frequency devices [1–3]. These devices grown on any substrates by metalorganic chemical vapor deposition (MOCVD) or molecular beam epitaxy (MBE) generate various kinds of defects such as point, line, and planar defects. These defects in GaN play an important role in their device applications for the electronic industry [4]. The reduction in density of defects leads to improvement of optical and electrical properties of GaN. Many experimental and theoretical investigations for defects, which affect the structural, electrical, and optical properties of GaN, have been reported in the literature [5,6]. In the case of planer defects in GaN, inversion domain boundaries (IDBs) in particular have been much studied, though their characteristics and origin are still a controversy [7–10]. The understanding of IDBs is important to characterize GaN films, because these affect the quality of GaN such as the surface structure and morphology. Though IDBs in GaN have been observed in various planes, many studies have been focused on the part of the boundary lying on the $\{10\bar{1}0\}$ planes. The configurations of IDBs are structurally described by changing the atomic positions at the interface, through an inversion and a translation. One configuration observed in most IDBs, that is termed IDB*, is related to a relative particular displacement of the inverse polarity domains on either side of the boundary. These IDBs have been shown to be electrically inert. Another IDB model, so-called Holt model, is characterized by the exchange of anion and cation leading to the formation of wrong bonds along the IDB plane which are electrically active.

In this Letter, the structures and the formation energy of IDBs are investigated using the Tersoff empirical potential. We calculate the atomic configurations of the Holt IDB induced by the interactions of the IDB* with the stacking faults. For the formation of IDBs, we also perform the growth simulation of GaN on GaN substrate with the IDBs.

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2. Simulation details

For the structural property of planar defects in w-GaN, we use a classical molecular-dynamics (MD) method based on the Tersoff empirical potential, where the atomic interactions are described by the potential energy function in the form of an interactive empirical bond order potential. Details of the Tersoff potential are described elsewhere [11,12]. Although these empirical methods cannot give accurate results compared to first principles methods, they can be applied to complex systems, which require a large number of atoms or longer calculations, such as the mutual interaction and the movement of defects.

We previously proposed the Tersoff potential parameters for GaN, shown in Table 1 [13]. For the reliability of the Tersoff potential parameters for w-GaN, we calculate the structural and elastic properties of w-GaN. These results are well agreement with other theoretical and experimental data, shown in Table 2.

The optimized structures of IDBs are calculated using a conjugate gradient method (with convergence limit of 4.33×10^{-5} eV/Å). For the growth simulation of GaN layers on GaN with the IDBs, the MD simulation is performed under constant volume and temperature conditions (i.e., canonical *NVT* ensemble) with Nose–Hoover thermostat. To integrate the Newtonian equations of motion, we use the fifth-order predictor-corrector algorithm with a neighbor list technique.

GaN substrate with the IDB* is constructed by a cube with $a = 12.76$, $b = 44.19$, and $c = 41.49$ Å. The temperature of GaN substrate is fixed at 1300 K. The 150 GaN molecules are emitted to the surface with a constant velocity of 500 m/s. The distance between the surface and the GaN molecule is 20 Å. The MD simulation is calculated for 350 000 iterations with a time step of 1.2×10^{-15} s at 1300 K and the periodic boundary condition is applied in a direction parallel to the deposition surface.

Table 1
Tersoff potential parameters for GaN

	Ga–Ga[a]	Ga–N	N–N[b]
A (eV)	2.8398×10^3	3.7321×10^3	1.1000×10^4
B (eV)	1.1479×10^2	2.3401×10^2	2.1945×10^2
λ (Å^{-1})	3.2834	3.6987	5.7708
μ (Å^{-1})	1.7154	1.9214	2.5115
β	2.3596×10^{-1}	1.0900×10^{-6}	1.0562×10^{-1}
n	3.4729	0.7873	12.4498
c	7.6298×10^{-2}	7.2239×10^4	7.9934×10^4
d	1.9796×10^1	1.0018×10^1	1.3432×10^2
h	7.1459	−0.5180	−0.9973
R (Å)	2.8	2.4	2.0
D (Å)	3.0	2.6	2.3

[a] Proposed by Nakamura et al. [14].
[b] Proposed by Kroll [15].

Table 2
Structural and elastic properties of w-GaN

	Present	Calculation	Experiment
a	3.208	3.196[a], 3.210[c]	3.190[d]
c/a	1.635	1.634[a], 1.631[c]	1.627[d]
E_{coh} (eV/atom)	−4.87	−5.27[a]	−4.53[d]
B (GPa)	187	213[a], 197[c]	188–245[d]
C_{11}	338	396[b], 350[c]	377[e], 390[f]
C_{12}	128	144[b], 140[c]	160[e], 145[f]
C_{13}	107	100[b], 104[c]	114[e], 106[f]
C_{33}	359	392[b], 376[c]	209[e], 398[f]
C_{44}	90	91[b], 101[c]	81[e], 105[f]
C_{66}	105	126[b], 115[c]	109[e], 123[f]

[a] LDA pseudopotential calculation [16].
[b] FP-LMTO LDA calculation [17].
[c] LDA pseudopotential calculation [18].
[d] Data reported in Ref. [19].
[e] Resonant ultrasound method [20].
[f] Brillouin scattering method [21].

3. Results and discussion

To investigate IDBs in w-GaN, the structures and the formation energy of $(10\bar{1}0)$ IDBs are first calculated. We consider four kinds of IDBs, which are grouped into IDB*-A, IDB*-B, Holt-A, and Holt-B. The optimized structures of IDB* and Holt type IDBs are shown in Fig. 1. The Holt IDBs show wrong bonds (Ga–Ga or N–N) by the exchange of anion and cation at the boundary, without any other translations in structure. The atomic structure of the IDB* is characterize by a $c/2$ translation to avoid the less favorable homoelemental bonds. As a result of simulations, the B type of IDBs leads to the geometrical distortion of w-GaN and has the structural instability, compared to the A type. Table 3 shows the formation energy of IDBs. These results are in agreement with other theoretical predictions. It is found that the structure of the A type is energetically more stable than that of the B type. However, Ruterana and Nouet have reported that the boundary plane can move from one type to the other of the same model despite the instability of the B type [23]. As compared the Holt type with the IDB*, the latter is energetically favorable in spite of fourfold and eightfold rings of bonds. Northrup et al. have also proposed that most of the IDBs correspond to the IDB* type and the formation energy for the IDB* is much less than for the other structures [24]. This indicates that the high energy cost of homoelemental Ga–Ga and N–N bonds may outweigh the cost of the structural transformation by fourfold and eightfold rings. Nevertheless, Holt IDBs, which are electrically active, are also observed experimentally [25,26].

Table 3
Defect formation energy (eV/Å^2) of IDBs in w-GaN

	Present	Calculation
IDB*-A	0.074	0.037[a], 0.025[b]
IDB*-B	0.127	
Holt-A	0.194	0.250[a], 0.167[b]
Holt-B	0.372	

[a] Stillinger–Weber potential [22].
[b] First-principles pseudopotential [24].