Atomic structures of twin boundaries in GaN

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The atomic structures of $(10\bar{1}1)$, $(10\bar{1}2)$, and $(10\bar{1}3)$ twins in the wurtzite gallium nitride have been studied by atomic computer simulation using an empirical interatomic potential of the Stillinger-Weber type. Distinct reference structures have been considered with respect to the type planes of the two adjacent crystals. The atomic structure of the twin boundaries was found to be dependent on these starting configurations. The lowest energy structure of the $(10\bar{1}3)$ boundary is composed by 6-coordinated channels whereas the $(10\bar{1}2)$ twin boundary can present three distinct structures composed by either 4-, 8-, or 5/7-coordinated channels separated by 6-coordinated channels. In both cases there is a mirror symmetry relating the two crystals. In the $(10\bar{1}1)$ twin the two structures of low energy do not exhibit mirror symmetry and present corrugated boundary planes.

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I. INTRODUCTION

Gallium nitride (GaN) is a semiconductor with great technological importance that has to be artificially produced. The growth has mainly been heteroepitaxial on several foreign substrates with different orientations including *a* plane $(1\bar{1}20)$, *m* plane $(10\bar{1}0)$, *r* plane $(01\bar{1}2)$, and *c* plane (0001) (for a review see, e.g., Ref. 1). The substrate employed determines the crystal orientation, polarity, polytype, the surface morphology, strain and the defects nature and concentration of the GaN film (for a review see, e.g., Ref. 2). The defects in the atomic structure should strongly influence the electronic properties of the GaN based devices and their optimal performances. A systematic study of the atomic structures of these defects contributes to the understanding of the behavior and performance of such devices at mechanical and/or electronic levels. The defects can be either localized or extended. The former, namely, point defects and their clusters, have been studied with great accuracy by first principle calculations.[3–8] The latter need to be reproduced in systems formed by thousands of atoms and therefore their study is hardly affordable by *ab initio* calculations. The use of empirical effective potentials allows us to perform such calculations. Among the extended defects existing in the grown GaN, threading dislocations and tilt boundaries are well recognized by the experimental observations[9,10] and their atomic structures have been recently simulated. Thus, the core shape and extension of $\vec{a}$ and $\vec{c}$ dislocations of both edge and screw character were reported and so were the atomic structures of several [0001] tilt boundaries with misorientation angles from 9.3° to 44.8°.[11,12] In addition, the various epitaxial relationships, induce the formation of other extended defects, such as twins, that causes serious problems in the semiconductor compounds as it reduces the single crystallite yield.[13] Whereas the most commonly observed twins in hexagonal-close-packed (h.c.p.) metals ($\{10\bar{1}1\}$,$\{10\bar{1}2\}$,$\{11\bar{2}1\}$, and $\{11\bar{2}2\}$ twins) have been extensively studied,[14–18] there is very little information on these twins in GaN. The only HREM published on twins in GaN to our knowledge concerns a cubic crystallite.[19]

In this paper we present the atomic structure of the $(10\bar{1}1)$, $(10\bar{1}2)$, and $(10\bar{1}3)$ twin interfaces in the GaN wurtzite. These twins include the $[11\bar{2}0]$ direction in the boundary and are likely to appear in the GaN grown on the $(11\bar{2}0)$ plane. A systematic procedure of creating and selecting the starting bicrystal structures of twin boundaries in a wurtzite structure is presented.

II. DETAILS OF CALCULATIONS

The relaxation procedure is based on the quench-molecular dynamic method. The relaxation finished when the thermodynamic temperature was smaller than 10^{-6} K.

A. Interatomic potential

The potential model employed is an empirical potential of Stillinger-Weber type that was previously used for the calculation of atomic structures in semiconductors.[20,21] The potential was adapted to take into account the different possible interactions, namely Ga-N, Ga-Ga, and N-N.[11] Although this potential can artificially favor overcoordination,[22] it has been successfully applied to describe the atomic structure, core energies, and the Peierls stress of dislocations,[11,23] structures of grain boundaries,[12,24,25] and dislocation-tilt boundary interactions[26] in GaN.

B. Simulation cells

The simulated system is a bicrystal with a periodic interface. The bicrystal has two regions: an inner relaxable region formed by 4000 mobile atoms and an outer fixed region. Periodic boundaries were applied in the directions along the interface and fixed in the direction perpendicular to the interface.

For a given twin plane, the structure of the twin boundary depends, on the one hand, on the chosen location of both, the lower plane of the upper crystal (P_λ) and the upper plane of the lower crystal (P_μ) and, on the other hand, on the relative position of the two crystals (for a comprehensive description see Ref. 27). Thus, in the simulation we considered all pos-

sible P_λ/P_μ combinations. In the $(10\bar{1}1)$, $(10\bar{1}2)$, and $(10\bar{1}3)$ orientations there are four distinguishable planes, each of them containing one of the four atoms of the basis of the wurtzite structure. This gives a total multiplicity of 4 $\times 4$ bicrystal structures created by bonding together all of the combinations of possible λ and μ surfaces. We recall that wurtzite structure can be imagined as two interpenetrating hexagonal substructures, one occupied by Ga atoms and the other by N atoms. The two substructures are shifted by approximately 3/8[0001], and the stacking sequence along [0001] is $\cdots AaBbAaBb\cdots$, where Ga atoms are in *A* and *B* planes and *N* atoms are in *a* and *b* planes. When the wurtzite structure is projected along $[11\bar{2}0]$, each stacking corresponds to a row of one of the four atoms of the basis. Then, the four possible P_λ/P_μ bicrystal structures formed from the $A(\lambda)$ surface are $A(\lambda)/A(\mu)$, $A(\lambda)/a(\mu)$, $A(\lambda)/B(\mu)$, and $A(\lambda)/b(\mu)$. Once the mirror twin is created, the other three are obtained by removing one, two or three P_μ planes. For each starting bicrystal configuration the lowest energy structure was identified in the corresponding γ surface calculated by applying relative displacements of the two half crystals parallel to the boundary.

III. RESULTS

A. $(10\bar{1}1)$ twin

Three relaxed structures of this twin projected along $[11\bar{2}0]$ are shown in Fig. 1. The four symbols represent the four atoms of the basis that are located in four layers along the normal to the twinning plane. The two first structures S_1 [Fig. 1(a)] and S_2 [Fig. 1(b)], were obtained with an $A(\lambda)/a(\mu)$ bicrystal configuration and the latter S_3 [Fig. 1(c)], from a $B(\lambda)/B(\mu)$ one. A single plane of atoms formed by the coalescence of two $(10\bar{1}1)$ planes forms the boundary of the structure S_1 whereas a corrugated plane marks the structures S_2 and S_3. The structure S_2 is related to the structure S_1 by a rigid body displacement in the direction of the twin plane with a clear effect on the mirror symmetry by changing the motif in one of the crystals. Our energetic calculations shown that structures with a corrugated boundary plane (S_2 and S_3) are energetically more favorable than the structure with a single plane boundary (S_1). These energies are 2709 mJ/m^2 for the structure S_3, 2753 mJ/m^2 for the structure S_2, and 3567 mJ/m^2 for the structure S_1. Other stable boundaries were found but the twin energy was higher than the low-energy structure given above.

B. $(10\bar{1}2)$ twin

We present in Fig. 2 the three atomic structures of low energy. The K_1 configuration contains a 4-coordinated channel [4-interface, Fig. 2(a)], the K_2 one, an 8-coordinated channel [8-interface, Fig. 2(b)], and the K_3 configuration, a 5/7-coordinated channel [5/7-interface, Fig. 2(c)]. The structures were obtained from a twin with mirror symmetry by removing one, two, or three $(10\bar{1}2)$ layers of atoms. Then, the mirror symmetry was recovered in the relaxation process.

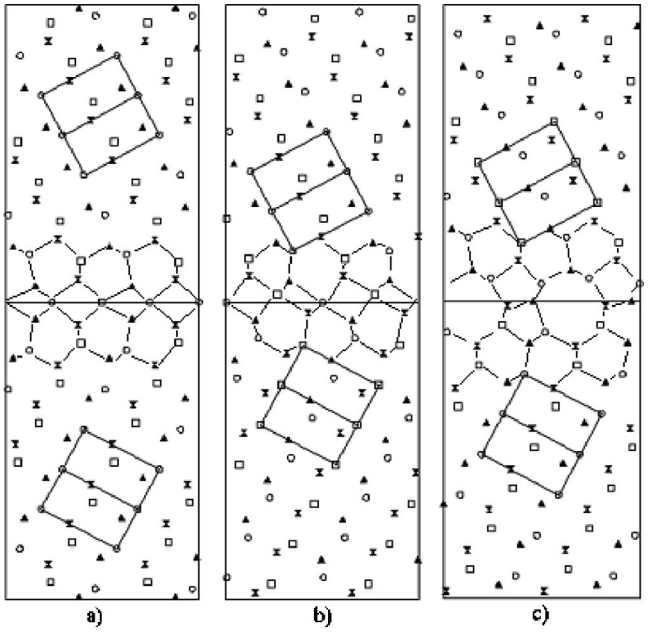

FIG. 1. Lowest energy structure of the $(10\bar{1}1)$ twin projected along $[11\bar{2}0]$. The four symbols represent the four layers in the stacking sequence. Hexagonal unit cells are shown in outline. Squares correspond to *A*-type layers, triangle to *a*-type, circles to *B*-type, and crosses to *b*-type layers in the stacking sequence of the wurtzite structure along [0001].

All these boundaries are marked by a single plane of atoms formed by the coalescence of two or three $(10\bar{1}2)$ planes that were distinct in the unrelaxed structures. The K_1 configuration was obtained from a $B(\lambda)/b(\mu)$ bicrystal structure and the K_2 and K_3 configurations from $b(\lambda)/A(\mu)$ and $b(\lambda)/b(\mu)$, respectively. The energetic calculations indicate that the 4-interface ($\Delta E = 1954$ mJ/m^2) is energetically more favorable than the 8-interface ($\Delta E = 2478$ mJ/m^2) and the

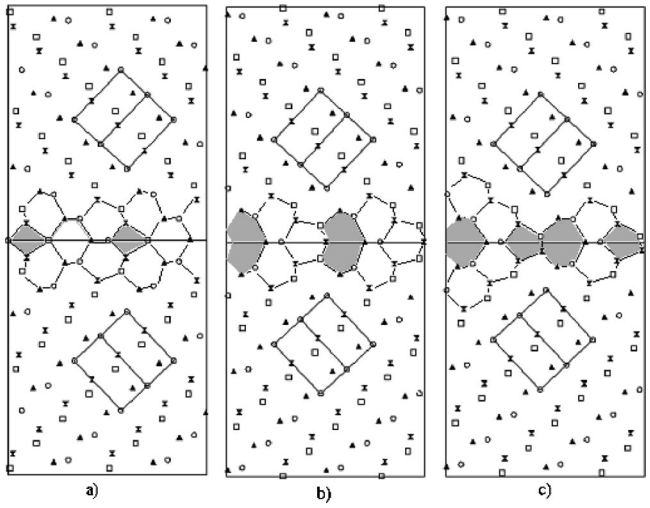

FIG. 2. Atomic structures of the $(10\bar{1}2)$ twin projected along $[11\bar{2}0]$. The structure in (a) exhibits a four-coordinated channel (4 interface), in (b) an eight-coordinated channel (8 interface), and in (c) five- and seven-coordinated channels (5/7 interface).

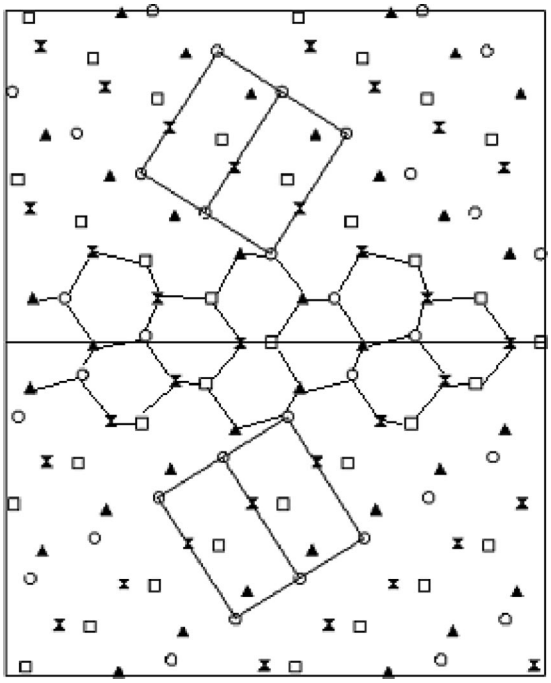

FIG. 3. Lowest energy structure of the $(10\bar{1}3)$ twin projected along $[11\bar{2}0]$.

5/7-interface ($\Delta E = 2809$ mJ/m^2). Notice that similar structural units (4-, 5/7-, and 8-coordinated channels) have been obtained for the [0001] tilt boundaries of low rotation angle. In that case it was found a direct relation of these structures and the three core structures of the $\bar{a}$ prism edge dislocation.[11]

C. $(10\bar{1}3)$ twin

Figure. 3 shows the low-energy structure obtained for this twin. A single plane of atoms formed by the coalescence of two $(10\bar{1}3)$ planes as in the previous cases marks the boundary plane. The relaxed structure was obtained from an $A(\lambda)/B(\mu)$ bicrystal configuration. It shows mirror symmetry and the structural units composing this boundary exhibit six-coordinated channels. The twin-boundary energy is 1302 mJ/m^2. Other stable boundaries were found but the twin-boundary energy was much higher. This energy is much lower than the values obtained for the low-energy structures of the $(10\bar{1}1)$ and $(10\bar{1}2)$ twins. This is in agreement with the fact that the 6-coordinated channels minimize the distortion of the tetracoordination.

IV. SUMMARY AND CONCLUDING REMARKS

We have simulated $(10\bar{1}1)$, $(10\bar{1}2)$, and $(10\bar{1}3)$ twins using an empirical potential of Stillinger-Weber type. For each boundary we have considered distinct reference bicrystal structures and we have calculated the corresponding γ surfaces to search all possible stable configurations. The core structure of the twin boundaries was found to be dependent on the starting bicrystal structure P_λ/P_μ. Although some starting configurations do not present an entirely symmetrical shape the mirror symmetry was recovered by rigid body displacements parallel to the twin plane and/or during the relaxation process. 4-, 8-, or 5/7-coordianted channels separated by 6-coordinated channels describe the $(10\bar{1}2)$ boundary whereas 6-coordinated channels uniquely composed the $(10\bar{1}3)$ boundary that is the one with lowest energy. The energy calculations show that the low-energy structures only exhibits a pure mirror symmetry for the $(10\bar{1}2)$ and $(10\bar{1}3)$ twins.

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