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The 60° basal dislocation in wurtzite GaN: Energetics, electronic and core structures

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ABSTRACT

We have carried out computer atomistic simulations, based on an efficient density functional based tight binding method, to investigate the core configurations of the 60° basal dislocation in GaN wurtzite. Our energetic calculations demonstrate that the glide configuration with N polarity is the most energetically favorable over both the glide and the shuffle sets in nitrogen-rich growth conditions. However, in the case of gallium-rich growth conditions, the shuffle configuration with gallium polarity becomes the most favorable. Otherwise, we found that all the four configurations of the 60° basal dislocation introduces both shallow and deep states but the glide configuration with N polarity, which introduce only shallow states.

1. Introduction

Gallium nitride along with its aluminum and indium alloys belong to the group III-nitride semiconductors [1]. These materials exhibit some unique physical properties [1], namely a direct bandgap, which make them technologically relevant [2]. Moreover, it was demonstrated that depending on the alloy composition; the direct bandgap varies continuously from about 0.7 eV to 6.2 eV, covering a wide wavelength range from red through yellow and green to blue and ultraviolet [2].

Most of gallium nitride used for optoelectronic applications is usually grown as thin films. The growth is achieved on thermally and structurally mismatched foreign substrates, by using hetero-epitaxial techniques [3]. This results in GaN layers with a huge content of structural defects, namely threading dislocations which penetrate vertically the whole layer and thus reach the active region of the building devices. Threading dislocations are present with a typical density of 10^{10} cm^{-2} [4] and were proven to have a harmful impact on the performances of the GaN based optoelectronic devices [5].

Wurtzite GaN layers were initially grown along the [0001] direction, also called polar direction [3]. This led to the fabrication of optoelectronic devices, based on heterostructures, which are strongly affected by spontaneous and piezoelectric polarization effects [6]. These effects are at the origin of the occurrence of a high internal electrostatic field which increases the separation between electrons and holes and thus reduces the overlap of their wavefunctions [6]. The latter causes a strong current dependence of the emission energy and a red shift of optical transitions as well as reduces the emission efficiency of optoelectronic devices [6]. The polarization-related effects in wurtzite GaN heterostructures can be completely avoided by adopting growth on alternative orientations. Hence, various growth directions were explored. These were the non-polar directions: $[11\bar{2}0]$, $[10\bar{1}0]$ and the semi-polar directions: $[10\bar{1}\bar{3}]$, $[10\bar{1}\bar{1}]$ and $[11\bar{2}\bar{2}]$ [7]. Then, GaN/AlGaN heterostructures grown along non-polar [8] or semi-polar [9] directions were proven to be free from polarization effects and thus demonstrate a clear improvement of their optical properties with respect to those elaborated along the polar direction.

The nature of threading dislocations contained in a wurtzite GaN layer is directly related to the direction of its growth. If the growth direction is [0001], i.e. the polar direction, the threading dislocations are perfect prismatic dislocations, which can be edge, screw or mixed [10]. However, if the growth direction is $[11\bar{2}0]$, i.e., the non-polar direction, the threading dislocations can be perfect or partial basal dislocations [10]. Perfect basal dislocations are

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screw and 60°-mixed, while partial basal dislocations are Shockley (edge, 30°-mixed), Frank and Frank-Shockley partials [11].

During the last decade, threading prismatic dislocations were extensively investigated in gallium nitride, at both experimental and theoretical levels [10]. For these dislocations, models for their core structures were proposed and their impact on the electronic properties of GaN was nearly elucidated [12–16]. The body of work dedicated to basal dislocations in GaN still insufficient compared to that to prismatic dislocations [10], while among basal dislocations, partials [17–20] were more investigated regarding the perfect ones [21–24]. The perfect screw dislocation was investigated atomistically and the energetic hierarchy of its core configurations was established by Belabbas et al. [24]. The perfect 60° dislocation was studied in cubic GaN by Blumenau et al. [25] but unfortunately no theoretical report exists for the wurtzite phase. At the experimental level, the perfect 60° dislocation was observed by using electron microscopy. By combining conventional transmission electron microscopy and cathodeluminescence measurements, Albrecht et al. [26] investigated the 60° dislocation in wurtzite GaN and analyzed its electronic and optical activities. They found it to be likely responsible for a parasitic luminescence around 2.9 eV. However, due the limited resolution of their used microscope, the previous authors were not able to establish if this observed behavior is that of a full or a dissociated dislocation. In a subsequent study, Niermann et al. [27] have observed a dissociated 60° dislocation by using high resolution transmission electron microscopy. The separation between the two resulting Shockley partials was found to be smaller than 2 nm. Such dissociation was further observed by Zakharov et al. [28].

In the present contribution, we have carried out computer atomistic simulations to investigate the core configurations of the 60° basal dislocation in GaN wurtzite. Besides their electronic and atomic core structures, we have also addressed the issue of their energetical hierarchy and its dependence on the growth conditions.

2. Models and simulation details

The 60° basal dislocation has a mixed character (edge and screw). In the wurtzite crystal structure, this dislocation is perfect and has its line along the $[1\,1\,\bar{2}\,0]$ direction and its Burgers vector is $1/3[2\,\bar{1}\,\bar{1}\,0]$ which has a magnitude equal to a (a = 3.18 Å stands for the basal lattice vector of GaN). The 60° basal dislocation may have several core configurations, which depends on the position of its center. If the latter is located between two narrowly spaced {0 0 0 1} planes, called the glide set, the dislocation will have a glide configuration. However, if the center of the dislocation is situated between two widely spaced {0 0 0 1} planes, called the shuffle set, the dislocation will have a shuffle configuration. As gallium nitride is a compound semiconductor, a glide (or a shuffle) core configuration may exists in two different polarities: gallium or nitrogen. This depends on the nature of the ending atom at the additional half plane, which is at the origin of the edge component of the dislocation.

The 60° basal dislocation was modeled atomistically by using the so-called supercell-cluster hybrid model [12–14]. Within this model the natural periodicity of the defect along its line direction is kept, while the lateral dimensions of model are taken finite and thus an amount of bulk material is included around the dislocation. This has to be large enough to prevent the spurious interaction that may occur between the model lateral's surface and the dislocation. Moreover, the atoms at the model's lateral surface (Ga/N) have to be saturated by fractionally charged (1.25e/0.75e) pseudo-hydrogen atoms which allow getting rid of dangling bonds and their associated unwanted gap states [12–14]. The supercell-cluster hybrids were at least doubled along $[1\,1\,\bar{2}\,0]$direction in order to take into account any possible reconstruction along the dislocation line. The size of the models considered here is ranging from 750 to 1000 atoms and their lateral extension is typically about 26 Å. Although the lateral extension of the model is finite, periodic boundary conditions were applied laterally to the dislocation line while including a 50 Å of vacuum. This was found sufficient to prevent interactions between the primary and image cells produced by periodic boundary conditions.

The initial positions of the atoms forming the dislocation were generated by using the displacement field given by linear elasticity theory [29]. The final positions were obtained through energetic calculations based on the so-called SCC-DFTB method, which is a self-consistent tight binding method based on density functional theory [30]. Within this method the total energy of the system is evaluated via the resolution of Kohn–Sham-like equations, where an approximate hamiltonian is adopted. The key feature behind the transferability of the SCC-DFTB method is the incorporation of a self-consistent procedure, at the Mulliken charges level, which allows for charge redistribution [30]. This is essential for the description of the different bonding states that may be involved in the core of dislocations in GaN (Ga–N, Ga–Ga, N–N and dangling bonds). Otherwise, the SCC-DFTB method is numerically very efficient as it makes possible to treat systems with thousands of atoms.

The equilibrium atomic positions were obtained through a minimization procedure based on the conjugate gradient algorithm where energies and forces are evaluated by using the SCC-DFTB method. During this step all the atoms, including those at the model's lateral surfaces, were allowed to relax freely. The equilibrium is reached when the maximum force acting on each atom of the system is well below 0.0001 a.u. Within these calculations the electronic valence wave function was expanded in a basis set of 14 contracted valence pseudo-atomic wave functions. This basis set includes 3d, 4s and 4p orbitals of gallium, 2s and 2p orbitals of nitrogen and 1s orbital of hydrogen. Each orbital is expanded in a convergent basis formed by 12 Slater-type orbitals. Hamiltonian and overlap matrix elements are evaluated within the Slater–Koster two-center approximation. The repulsive interatomic potential is generated by fitting DFT based local density-approximation (*LDA*) calculations that are performed for different suitable reference systems [31].

The adopted (Ga, N) parameterization of the SCC-DFTB method allows achieving good accuracy for structural and elastic properties of bulk wurtzite GaN. Calculations carried out here, gave lattice parameters: a = 3.178 Å and c = 5.214 Å, in good agreement with experimentally observed values of a = 3.190 Å and c = 5.189 Å [32]. This led to a Ga–N bond length of 1.947 Å. For the bulk modulus we have obtained the value of 189 GPa, which is very close to the available experimental one of 188 GPa [33,34]. Furthermore, the elastic constants were computed and the following values were obtained: C_{11} = 388 GPa, C_{12} = 106 GPa, C_{13} = 62 GPa, C_{33} = 432 GPa, C_{44} = 114 GPa, C_{66} = 141 GPa. These are in good agreements with the published experimental values [35]. Finally, by evaluating the Mulliken charges on each atom, a charge transfer of 0.56e was quantified from the Ga to N atoms, resulting in a polar bonding character. Otherwise, the SCC-DFTB method has proven to be an efficient tool for investigating atomic and electronic structures of defects in wurtzite GaN, like dislocations [12–14] and grain boundaries [36].

3. Results and discussion

For the 60° basal dislocation, we have considered four core configurations: a shuffle configuration with nitrogen polarity (60°-S_N),