Structural and Electronic Properties of Threading Screw Dislocations in GaN

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GaN is a promising material for applications to power electronics devices with its favorable high field and thermal transport properties [1]. However, the presence of high density of threading dislocations ($> 10^8$ cm^{-2}) in GaN is problematic. They limit the performance of power devices by reducing the photoluminescence intensity and the electron mobilities, and may end up leading to premature device breakdown. Therefore it is important to evaluate their impact on device performance and reliability. Here we focus on threading screw dislocation, which is a non-radiative recombination center with deep electronic states in the band gap, with different types of core structures and evaluate their energetics by the first-principles method using hybrid Hartree-Fock density functionals.

The core structure of threading screw dislocations in GaN is still under debate. Recently a new configuration of screw dislocation core is introduced by Belabbas et al. [2], where the dislocation line is located at the middle of bonds connecting two adjacent projected hexagons ("B" core), while it is located at the center of projected hexagon in the conventional screw core configuration ("A" core, see Fig. 1). We have investigated this new "B" full core structure as well as several types of "A" core structures: full (6:6), open (0:0), Ga-filled (6:0) and N-half-filled (6:3) structures, where the numbers in parenthesis, (n_{Ga}:n_N), denote the numbers of Ga and N atoms remaining in the core region.

Our calculations are performed using the projector augmented wave method with the Perdew-Burke-Ernzerhof (PBE) functional and Heyd-Scuseria-Ernzerhof (HSE) functional [3] implemented in the VASP code [4]. Ga 3d electrons are considered as valence electrons and energy cutoff is set to 425 eV. Our fully periodic supercell accommodates dislocation dipole and contains up to 288 atoms of Ga and N. The supercell for "A" open core structure is shown in Fig. 2.

Relative formation energies are shown in Fig. 3, which are calculated based on the Northrup formalism [5] and are expressed as a function of the Ga chemical potential (μ_{Ga}). In N-rich growth condition (at -1.17 eV) the most stable structure is the "B" full core. This result is consistent with the one by Belabbas et al., who insist it is the most stable under any growth conditions within their calculations based on local density approximation [2]. However, in Ga-rich growth condition (at 0 eV), contrary to the findings by Belabbas et al., the most stable structure is the Ga-filled (6:0) "A" core, which is originally proposed by Northrup [5]. We will show the detailed structural properties of these stable dislocation configurations and the electronic properties including their band structures calculated using the HSE hybrid functional (see Fig. 4).

REFERENCES

[1] J. L. Hudgins, G. S. Simin, E. Santi, and M. Asif Khan, *An Assessment of Wide Bandgap Semiconductors for Power Devices*, IEEE Trans. Power Electronics **18**, 907 (2003).

[2] I. Belabbas, J. Chen, and G. Nouet, *A new atomistic model for the threading screw dislocation core in wurtzite GaN*, Computational Materials Science **51**, 206 (2011).

[3] J. Heyd, G. E. Scuseria, and M. Ernzerhof, *Hybrid functionals based on a screened Coulomb potential*, J. Chem. Phys. **118**, 8207 (2003); **124**, 219906(E) (2006).

[4] G. Kresse, and J. Furthmüller, *Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set*, Phys. Rev. B **54**, 11169 (1996).

[5] J. Northrup, *Theory of intrinsic and H-passivated screw dislocations in GaN*, Phys. Rev. B **66**, 045204 (2002).
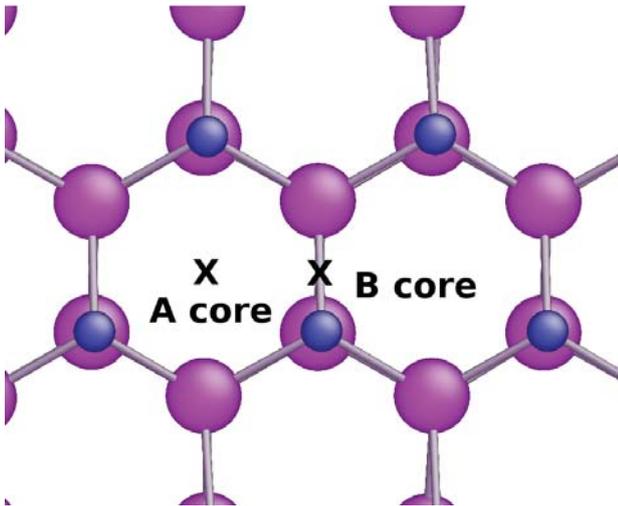
Fig. 1. Two different core configurations for threading screw dislocation projected onto the (0001) plane. The positions of dislocation lines are denoted by the cross marks. The "A" core is located at the center of projected hexagon and "B" core is at the middle of bonds connecting two adjacent hexagons.
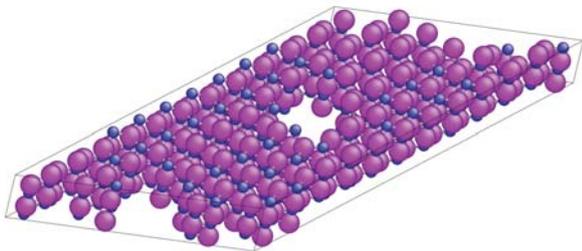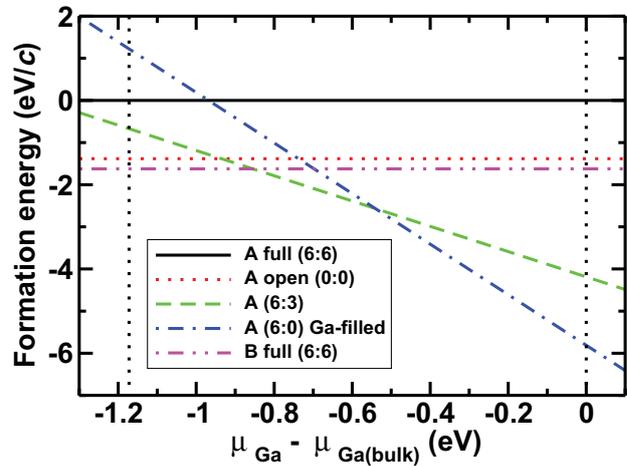

Fig. 3. Relative formation energies of different core structures as a function of the Ga chemical potential. The dotted vertical bars at 0 eV and -1.17 eV denote the Ga-rich limit and the N-rich (Ga-poor) limit, respectively.
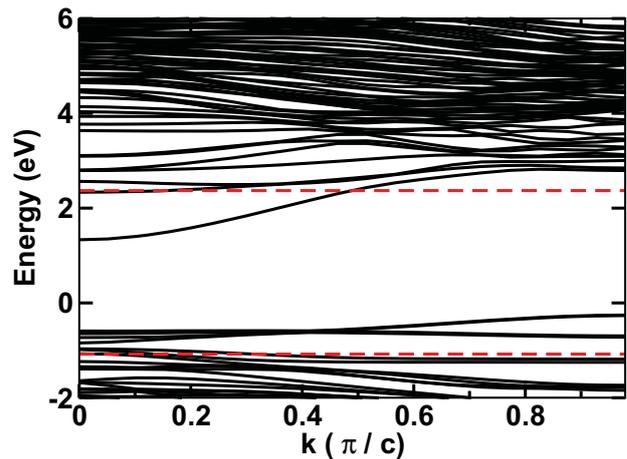

Fig. 2. Three dimensional view of our periodic supercell containing two open core screw dislocations.

Fig. 4. Band structures of screw "B" core configuration along the [0001] direction calculated by HSE. Fermi energy is located at 0 eV. The red dashed lines at -1.1 eV and -2.4 eV correspond to the valence band maximum and the conduction band minimum of bulk (without dislocation) GaN, respectively.