Self-regulated charge transfer in c-axis-oriented GaN nanorods and the repulsive interactions among them

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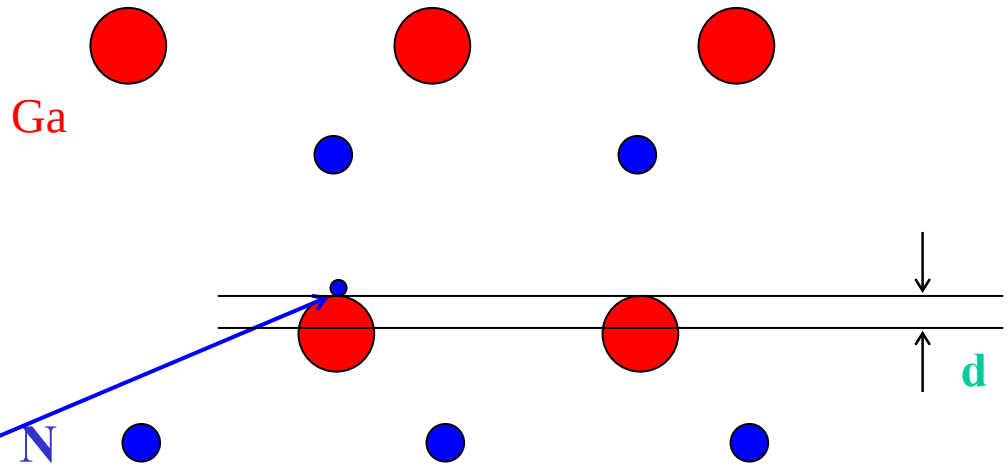
(NSC-

Motivation:

- **1. Polar wurtzite GaN(0001) nanorods are composed of an array of dipolar Ga-N bilayers, which gives rise to an electrostatic potential difference across the rod that tilts the energy bands.**
- **2. When the rod is long enough, the potential difference causes electrons to move from the N^--end to the Ga^+-end to regulate the potential difference.**
- **3. A given nanorod is an electric dipole. Parallel dipoles repel each other, so that nanorods have repulsive interactions among them, which may stablize GaN nanorod/wire formation.**

Origin of the polarization envisioned by Bernardini, Fiorentini and Vanderbilt [1]



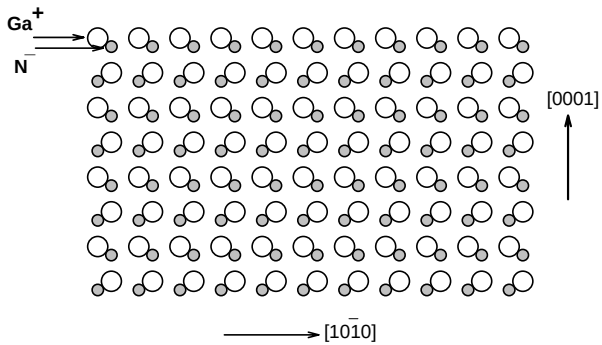
- **Negative charge center**

  d=(*u*-0.375)c

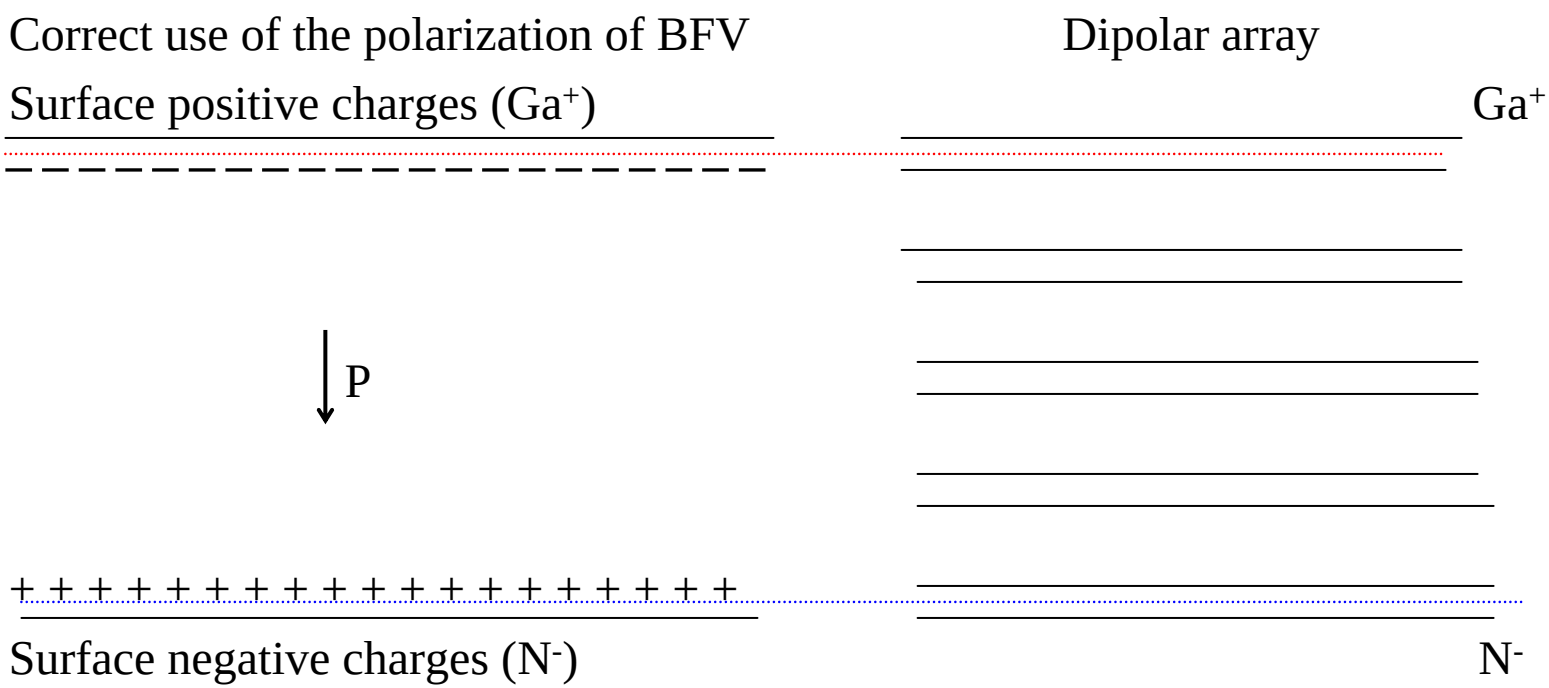
When *u*=0.3764, P=-0.028 C/m² (calculated: -0.029 C/m² [1])

[1] Phys. Rev. **B56**, R10024 (1997)

Side view of wurtzite GaN(0001)



Comparison between two views of charge arrangement in GaN(0001)



Surface charges are **much larger than** the **compensation charges of polarization**

Problems of the "spontaneous" polarization of Bernardini, Fiorentini and Vanderbilt

- **1. "Spontaneous" is not a proper description of this polarization.**

- **2. The –0.029 C/m2 polarization is due to the small deviation of u from 0.375. The compensating surface charge density of this polarization is only 0.0005 e/ao2, which is negligible comparing to Ga/N surface charge density.**
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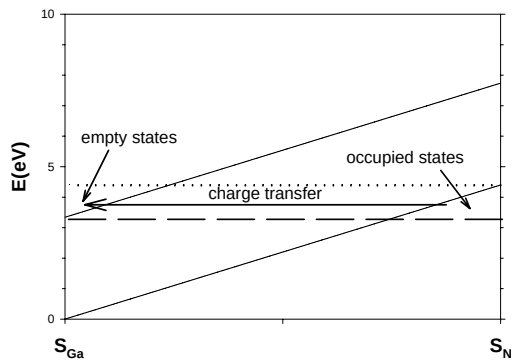
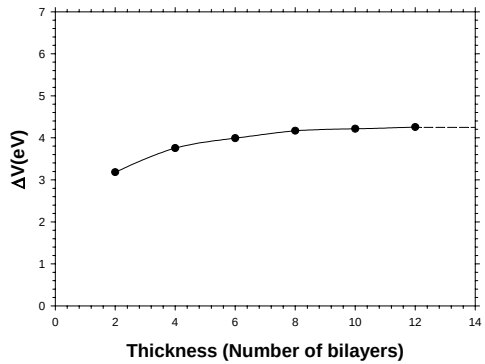
- **3. Due to the long-ranged nature of the Coulomb potential, real films, even in the interior of the film, don't have the symmetry of the infinitely extended bulk system, which doesn't have any surface and surface charges.**

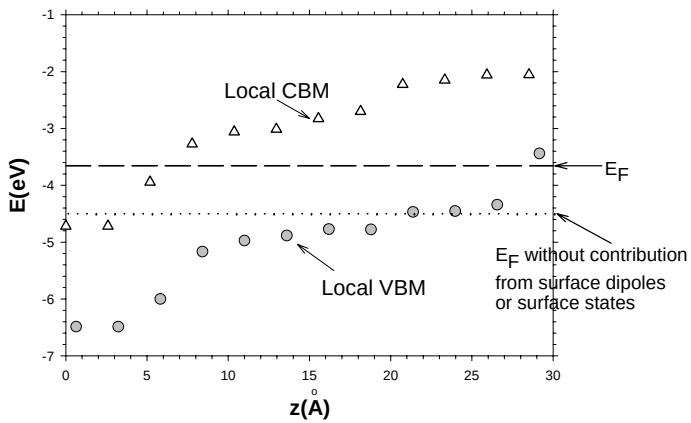
Tilt of energy bands in the GaN(0001) film/rod without across-film charge transfer



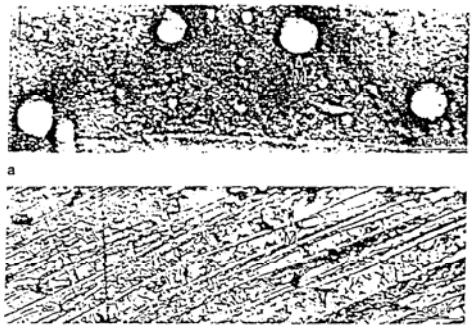
Potential energy difference across wurtzite GaN(0001) films/rods



Local valence band maxima and conduction minima in the 12-bilayer thick (long) wurtzite GaN(0001) film (rod)



Hollow-core Screw Dislocations



a

b

Fig. 1. (a). A back-reflection topograph (reflection vector g = 00024, wavelength λ = 0.125 nm) recorded from the as-grown surface, which reveals the micropipe (M) as well as elementary Burgers vector screw dislocations (S), (b). The NOM micrograph recorded from the same region.

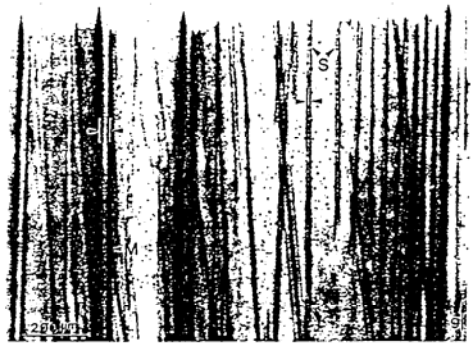


Fig. 2. A transmission topograph (g = 0006, λ = 0.075 nm) recorded from the (11 $\bar{2}$ 0) wafer. M indicates micropipe, and S indicates elementary screw dislocations.

In this study, quantitative analysis of micropipes as well as other screw dislocations along the c axis is reported, emphasizing on the determination of the magnitude of the Burgers vector of the screw dislocations, b, and the diameter of the associated hollow cores, D, and the correlation between these quantities in order to test the validity of Eq. (1).

EXPERIMENTAL PROCEDURES

A wafer with [11 $\bar{2}$ 0] surface normal was prepared from the 6H-SiC crystal boule grown by Cree Research. Synchrotron topography was performed at the Brook Synchrotron Topography Facility, Beamline X-19C, at the National Synchrotron Light Source (NSLS), at the Brookhaven National Laboratory (BNL). Several diffraction geometries, including the back-reflection, the transmission projection, and the transmission section, were employed to image the screw dislocations in the wafer. The SEM performed on a JEOL JSM-5300 Scanning Microscope was used to image the hollow cores of the screw dislocations on the as-grown surface. Nomarski optical microscopy (NOM) was used to reveal the overall relief of the as-grown surface, and help to locate the micropipes in the corresponding SEM and SWBXT images.

RESULTS

Determination of Burgers Vectors

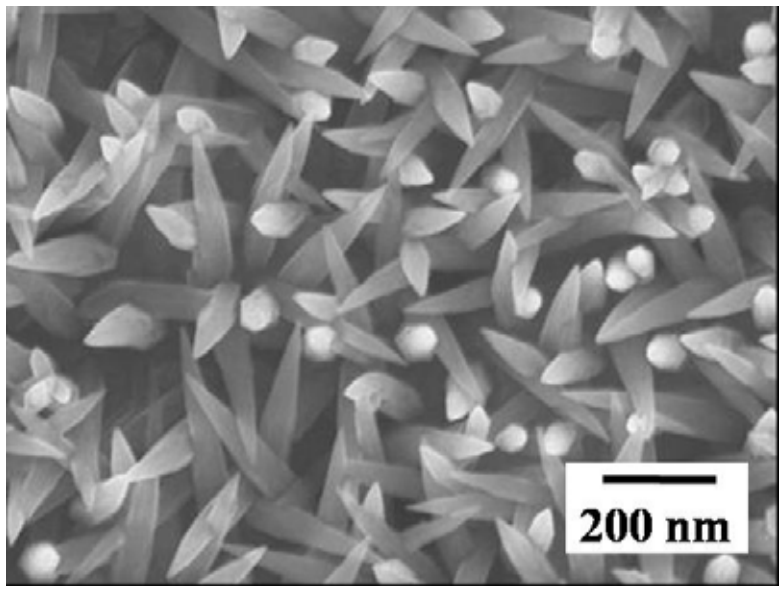
Four SWBXT methods have been employed to determine the magnitude of the Burgers vector of screw dislocations. Two of the four methods can also determine the sense of the Burgers vector. Each method will be presented and discussed in detail:

Method A: Measurement of Diameters of Dislocation Images in Back-Reflection Topographs

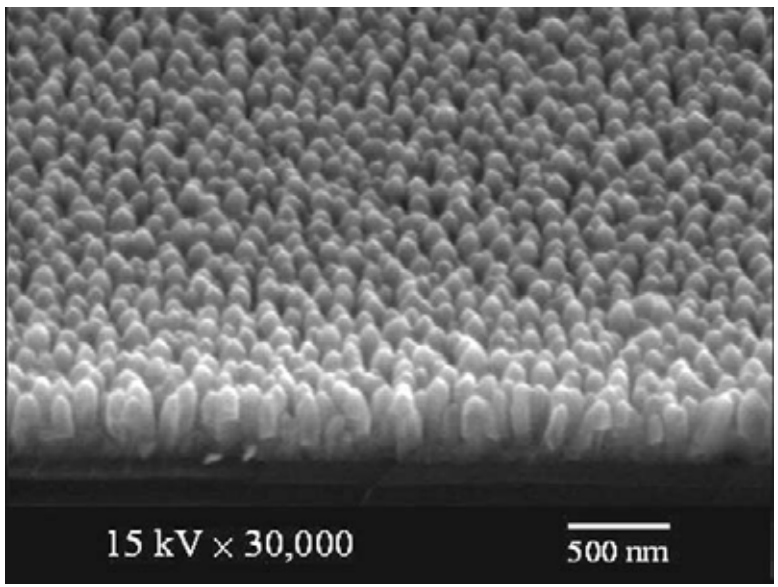
X-ray topographs recorded in the back-reflection geometry were found to be particularly suitable for imaging micropipes as well as other screw dislocations roughly parallel to the c axis. Figure 1a shows a back-reflection topograph recorded from the as-grown surface, where the large circular contrast features indicated by **M** (appearing as black rings with white centers) on the topograph coincide exactly with the positions of the emergent ends of micropipes. There are also many smaller such circular features (**S**), each with approximately the same size, observed on the back-reflection topograph. This kind of diffraction contrast has been discussed in Ref. 8. Figure 1b is an accompanying NOM micrograph recorded from the same region, showing numerous surface steps.

In direct images such as those shown in Fig. 1a, according to kinematical diffraction theory, the diameter of the circular image is proportional to the magnitude of Burgers vector of the screw dislocations.[9] Assuming that the smallest circular contrast features are associated with screw dislocations of elementary Burgers vector in 6H-SiC (usually $|b| = 1c$, c = 1.517 nm), then the magnitude of Burgers vector of all screw dislocations can be determined by calculating the *ratio* of the diameter of the particular dislocation image to that of the smallest one. In Fig. 1a, the micropipe labeled as M has Burgers vector magnitude of about $3c$ to $4c$.

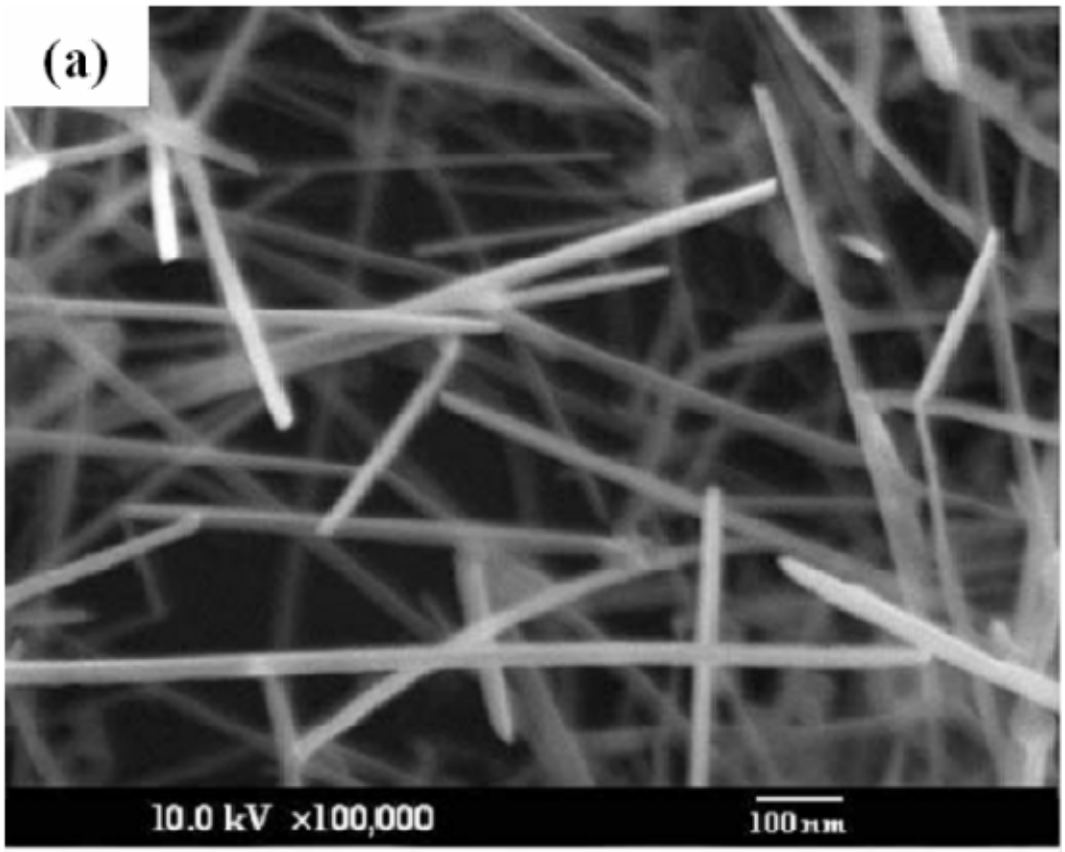
AlN nanotips



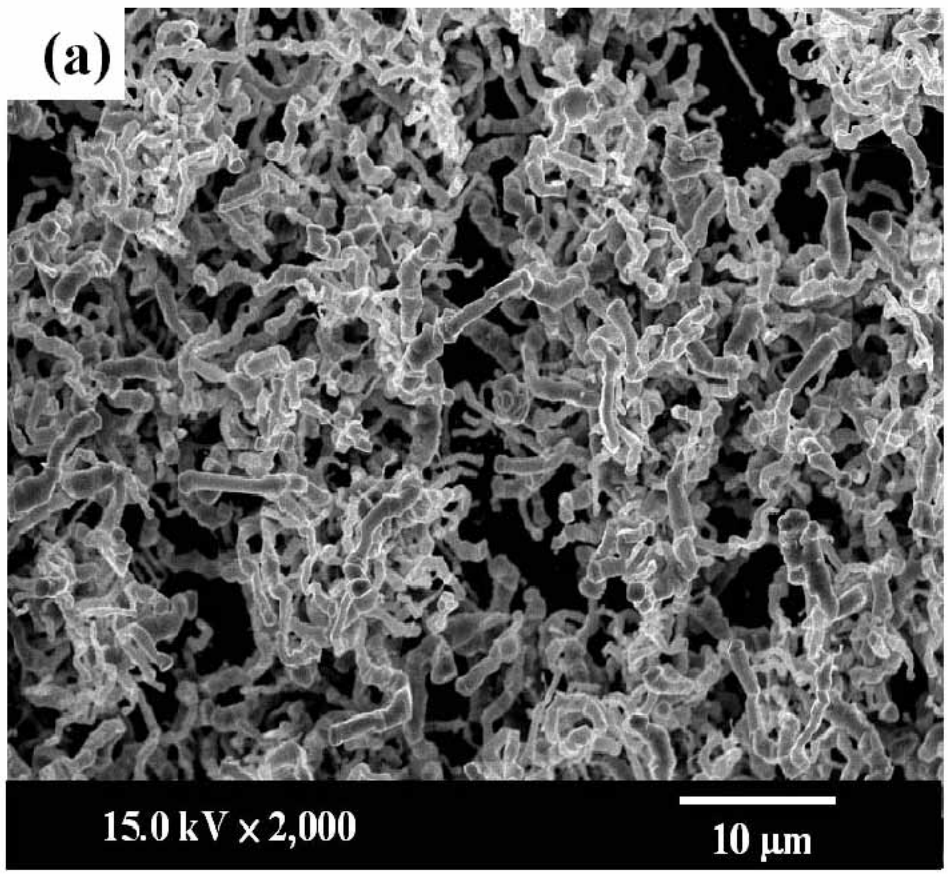
ZnO nanorods



GaN nanowires



GaN (tangled) nanowires



Relation between ionicity and crystal structure

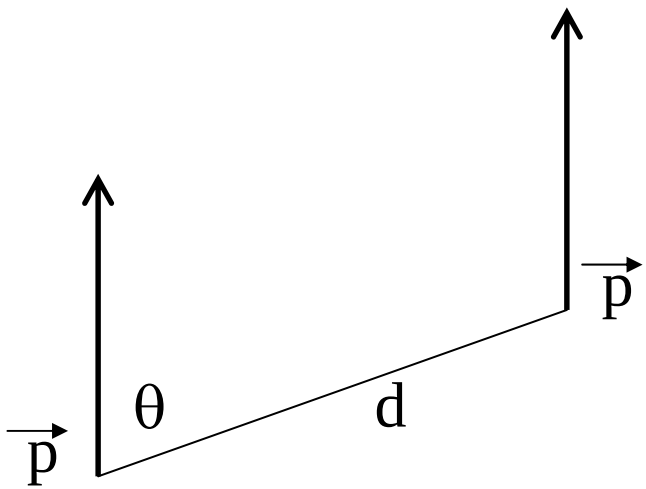
- Relatively low ionicity: zinc-blende structures
  e.g. GaAs, InAs, InSb, ZnTe, etc.

- Relatively high ionicity: wurtzite structure
  e.g. ZnO, GaN, AlN, etc.

- Very high ionicity: rock salt structure
  e.g. NaCl, KCl, CsF, etc.

Dipole-dipole interactions

- For parallel dipoles



$U_{dipole\text{-}dipole} = p^2(1-3\cos^2\theta)/d^3$

When $\theta = 90^o$, $U_{dipole\text{-}dipole} = p^2/d^3 > 0$---repulsive

Schematic drawing of a GaN nanorod bunch

Repulsive dipole-dipole interactions