OPTICAL SIGNATURE OF THE GaN (10$\bar{1}$0) SURFACE

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ABSTRACT

We present a theoretical study of the optical properties of the GaN (10$\bar{1}$0) surface. We employed a semi-empirical tight-binding method to calculate the surface electronic structure. The parameters were adjusted to reproduce the correct band structure of the bulk wurzite GaN. These parameters were interpolated to the surface using Harrison's rule. From the surface electronic structure the surface dielectric response was obtained. The dielectric response is analized in terms of surface-surface, and surface-bulk electronic transitions.

INTRODUCTION

The study of the optical and electronic properties of Gallium Nitride (GaN) has gained importance due to its potential application in near-ultraviolet opto-electronic devices [1,2]. GaN has a direct gap of 3.4 eV and at ambient conditions it crystalizes in the wurtzite structure, or in some cases, like thin films of GaN, the zinc-blende structure is obtained [3]. The bulk properties (electronic and optical) have been known for some time now. Bloom et al. [4] measured the reflectivity and calculated the band structure and reflectivity using an empirical pseudopotential method. It is not until very recently that systematic studies of the surface reconstruction of GaN were done. Jaffe et al. [5] studied the anomalous surface relaxation of GaN (10$\bar{1}$0) and (110), using an *ab initio* Hartree-Fock method. The equilibrium geometries for the principal nonpolar cleavage faces of GaN, are characterized by very small surface bond rotations and large surface and back bond contractions ($\sim$ -7%). Here, we use these results for the atomic structure of the GaN (10$\bar{1}$0) surface to study its optical properties.

MODELS AND METHOD OF CALCULATION

The GaN (10$\bar{1}$0) surface was modeled using a slab of 8 bi-layers, yielding a free reconstructed surface on each face of the slab. The thickness of the slab is large enough to decouple the surface states at the top and bottom surfaces of the slab. Periodic boundary conditions were employed parallel to the surface of the slab to effectively model a two dimensional crystal system. The x direction on the surface plane corresponds to the minor axis of the bulk wurzite unit cell, since the y axis corresponds to the long axis of the bulk unit cell. The calculations are done taking 32 atoms in the slab. The atomic coordinates of the two first layers were obtained from Reference [5], that utilizes an *ab initio* Hartree-Fock approximation, using linear combinations of Gaussian orbitals. The surface reconstruction is then characterized by no surface bond rotation and large surface and back-bond contraction.

To calculate the optical properties of the system, we generate the electronic level structure of the slab using a well known parametrized tight-binding approach. This method employs a sp^3s^* atomic-like basis, that provides a good description of the conduction band of semiconductors. The parameters for the GaN crystal with a wurzite unit cell were fitted to reproduce

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Table 1: Tight-binding interaction parameters for GaN

V_{ss}	-1.93		
V_{sp}	2.516	V_{ps}	-3.34
V_{pp_σ}	3.99	V_{pp_π}	-1.0925
V_{s^*p}	1.08	V_{ps^*}	-1.33

the bulk band structure reported on Refs. [4,6,7]. The values of the orbital energies for Ga are $\epsilon_s = -10.7806$eV, $\epsilon_p = 0.897$eV, $\epsilon_{s^*} = 11.5150$eV, and for N are $\epsilon_s = -0.5494$eV, $\epsilon_p = 5.6019$eV, and $\epsilon_{s^*} = 9.1850$eV. The parameters of tight-binding interactions are listed in Table 1. For the surface, we interpolated the parameters using Harrison's rule of $1/d^2$, where d is the bond length of any two first-neighbor atoms.

The optical properties of the surface region are determined by its dielectric function $\epsilon_s(\omega)$. We calculate the imaginary part of the average slab polarizability, which is related to the transition probability between eigenstates induced by an external radiation field. The surface dielectric response was obtained substracting the bulk dielectric response from the slab dielectric function. Here, the thickness of the surface layer of about 2.5 Å, was cosidered. Only two additional parameters to those of the tight-binding Hamiltonian were needed in order to reproduce the bulk dielectric function. These parameters are the so-called intra-atomic sp and s^*p dipoles, with best fitted values of 0.255 Å and 0.878 Å, respectively. The details of the calculation are fully explained in Ref. [8].

RESULTS AND DISCUSSION

Bulk properties

The bulk band electronic structure of GaN is shown in Figure 1. The tight- binding parameters were adjusted to fit the band structure of Refs. [4,6,7]. The direct gap at the Γ point has a value of 3.6 eV, which is similar to the value found theoretically and experimentally [4,6,7]. We observed that the calculated electronic structure is very similar for the valance states to those reported in Refs. [4,6,7], while some descrepancies are found for the conduction states. This is expected since previous theoretical formalisms had not taken into account an extended basis to describe correctly the conduction states. Notice that large cutoff energies are necessary in order to obtain a complete basis set using plane waves.

The anisotropic dielectric function of the bulk GaN was obtained using the calculated electron levels at 5808 points on the irreducible Brillouin zone. Then, the reflectivity transversal and parallel to the long axis of the wurzite unit cell is calculated. We show in figure 2 the reflectivity as a function of the frequency. These calculations are in agreement with those presented by Bloom et al. [4] using an empirical pseudopotential method. Compared to the experimental results [4], the reflectivity spectra of Figure 2 is in agreement in regard to the energies and relative shape of the peaks. The agreement holds up to an energy of ~ 8 eV due to experimental limitations reported by the authors [4]. Furthermore, our method of calculation for the optical properties was tested by comparing the zero frequency dielectric function with experimental values. The theoretical prediction gives a value of $\epsilon(0) = 5.4$ while the experimental values are in the range of 5.2 – 5.8 [4].

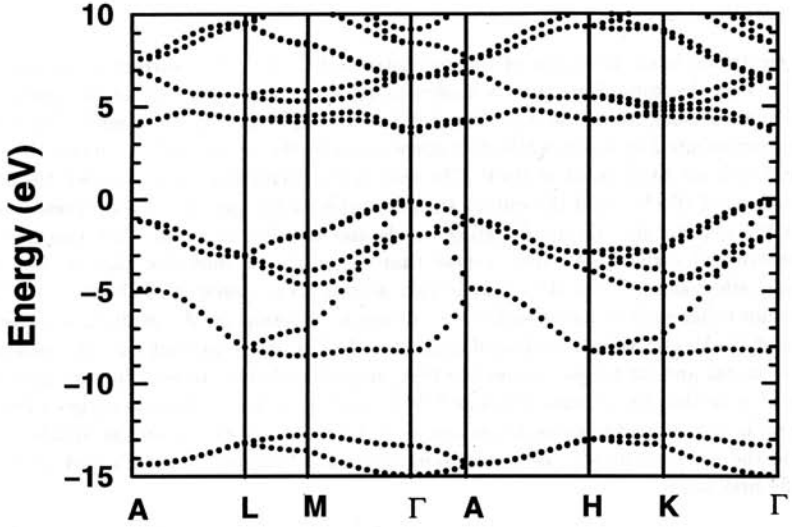

Figure 1: The bulk band electronic structure of wurzite GaN.

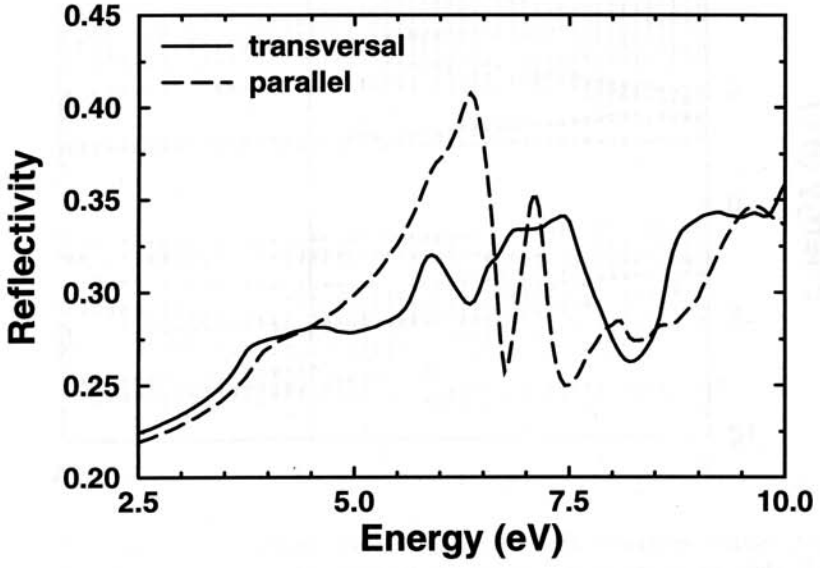

Figure 2: Reflectivity of bulk GaN for an external field transversal to the long axis (solid line) and for an external field parallel to the long axis (dashed line).

Surface properties

The electronic band structure of the reconstructed GaN $(10\bar{1}0)$ surface is presented in Figure 3. The electronic structure is shown along the main directions of the irreducible surface Brillouin zone, from Γ to J (x direction), and from J to K (y direction). The surface states are represented by stars, while dots correspond to the projected bulk states. The top of the bulk valence band is set at 0 eV. The calculated Fermi level is in between the top of the valence band (0 eV), and the empty surface states in the gap at 2.7 eV. These surface states in the gap are due to the dangling bonds and backbonds on the first two layers of the reconstructed surface. We can observe that along $J - K$ direction they do not show disperssion, since along $\Gamma - J$ they split in two, showing a disperssion of about 1 eV. There are also some other surface states within the valence band along the $J - K$ direction at about -1.3 eV and -2 eV, also with a backbond character. In Fig. 4, we present the total electronic density of states and its projection on the first, second and third layers. In this figure it is easier to observe that the surface states at 2.7 eV are due to the backbonds between the first and second layers, while the extended states from 2.7 eV to 3.7 eV are on the first layer and are due to the dangling bonds. We can also observe surface states at -1.3 eV and -2 eV that are on the first layer.

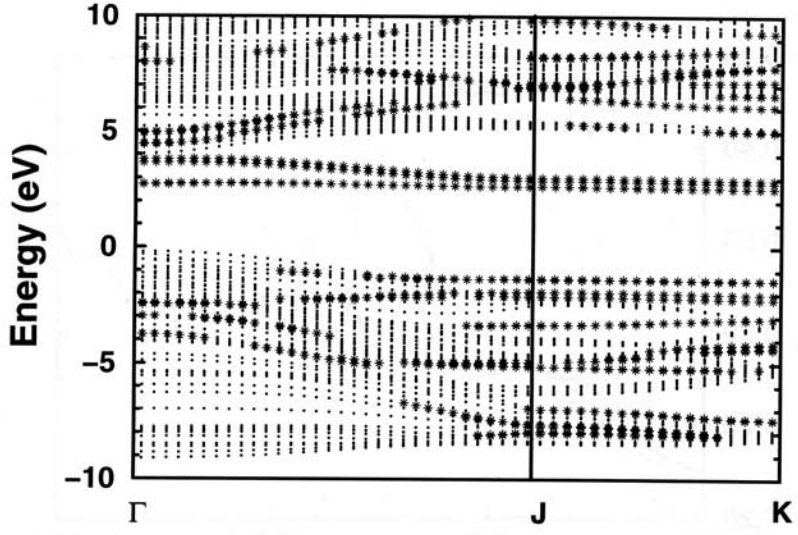

Figure 3: Surface electronic structure along the main symmetry directions of the surface unit cell. Dots correspond to the projected bulk states, while stars represent surface states. Resonance states embedded in projected bulk bands are also represented by stars.

The imaginary part of the average polarizability of the slab was obtained using the electron levels calculated at 4900 points distributed homogeneously on the irreducible surface

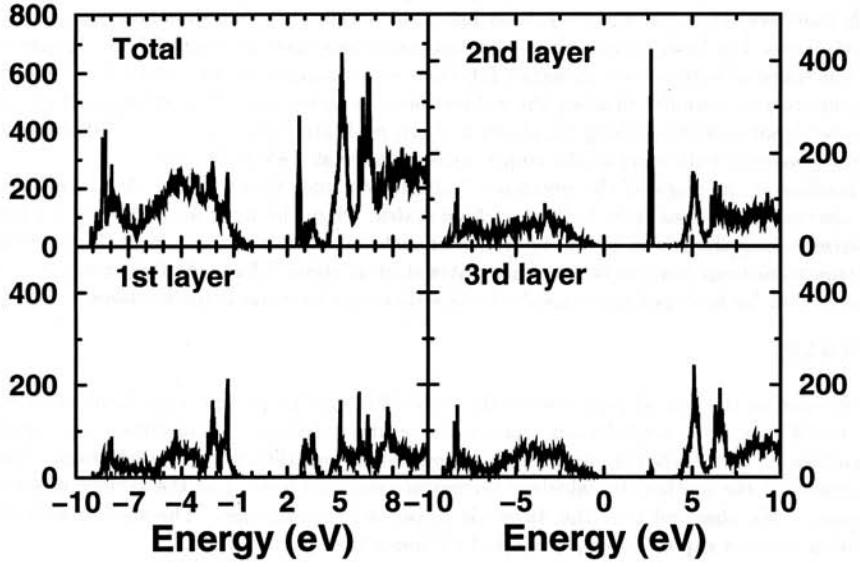

Figure 4: Calculated density of states for (a) total, (b) projected on first layer, (c) on second layer, and (d) on third layer.

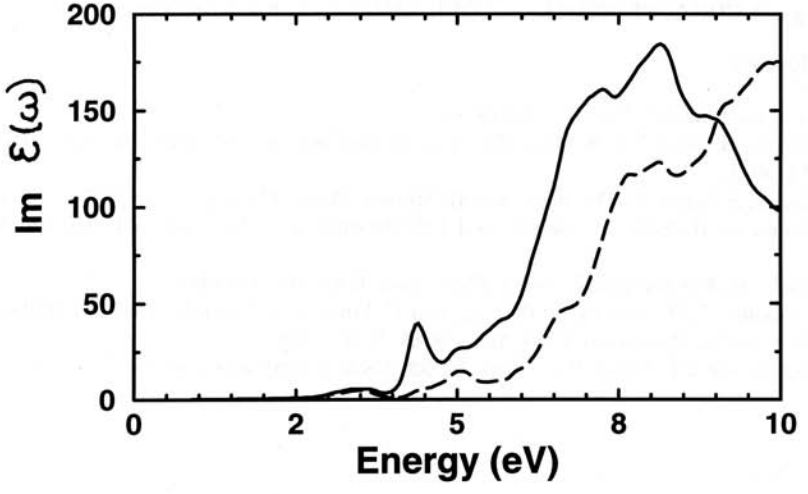

Figure 5: Imaginary part of the surface dielectric response. Solid line corresponds to light polarized along the x axis, while dashed line corresponds to light polarized along the y direction.

Brillouin zone. Figure 5 shows the imaginary part of the surface dielectric function, for both transverse (along x direction, solid line) and parallel (along y direction, dashed line) polarizations. For both polarizations, electron transitions start at about 2.7 eV. In general, the line shape of both surface dielectric functions is very similar up to about 8.5 eV, but the response to an external field along the x direction is more intense. At an energy of 4 eV, the transveral polarizability (along x), shows a sharp peak attributed to the optical transition from the valence bulk band to the empty surface states at 4 eV at Γ point.

Looking at the origin of the electron transitions one finds that from 2.7 eV to 4 eV there are electron transitions from bulk to surface states, while the peak at 4 eV only for light polarized along the x axis is due to transition between surface states. In both directions, electron transitions from surface to bulk states start at about 5.5 eV. At this energy, we can observe that for both polarizations the surface dielectric function is more intense.

SUMMARY

We studied the optical properties of the GaN $(10\bar{1}0)$ surface using a tight-binding formalism based on a sp^3s^* orbital basis. As a test, we first calculated the electronic and optical properties of bulk GaN that agree with experimental and theoretical observations. Then, we employed the method to calculate the surface electron levels and the surface dielectric response. We observed that the dielectric response is anisotropic. The surface dielectric function shows a gap of 2.7 eV, which is 1 eV lower than the bulk gap.

ACKNOWLEDGMENTS

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