Atomic and electronic properties of GaN nanowires

T. R. Vilela and H. W. Leite Alves
DCNAT, Universidade Federal de São João Del Rei, MG, Brazil

In the past decade, the GaN-based optoelectronic industry has grown rapidly. More recently, various forms of GaN nanomaterials such as nanorods and nanowires have attracted a great deal of attention as these nanosized GaN materials are expected to exhibit superior optical and electrical properties that may greatly extend applications of GaN-based materials. However, it is well known that the wurtzite phase of GaN is more stable than the zincblende one, which does not have induced dipoles in its structure and is preferable for the devices. Despite the fact that the electronic structure of these nanostructures have been extensively studied by applying hydrogen saturators to avoid surface effects in the calculations, little is known about how this system behaves when these hydrogen saturators are absent, i.e., how are the effect of the surface states on the electronic structure of these nanostructures. Moreover, it is not known if the zincblende modification of the nanowires can be, or not, more stable than the wurtzite phase. In order to complete the missing information about the electronic structure of these systems, we have show in this work, by using the Density Functional Theory (DFT) within the Local Density Approximation (LDA), gradient conjugated techniques, the Tight-Binding method (DFTB) [1], together with the supercell models, our preliminary results of the structural and electronic properties, as well as the formation energy of both the wurtzite GaN (0001) and zincblende GaN (111) nanowires with several diameters. Our calculations started with nanowires saturated by H atoms, and finished by removing these H atoms. We have analyzed the changes in the bond-lengths, bond-angles, as well as in its total energy, before and after the absence of the H saturators. Our results are in very good agreement with the available experimental data and other theoretical calculations, whenever these comparisons are possible. Based on our results, we have speculated about the effect of the surface states on the electronic structure of these nanowire systems, once they induce interesting facets on their lateral walls. Moreover, we have discussed whether a crystalline phase transition from wurtzite modification to the zincblende one can occur in these systems. Keywords: Structural properties, electronic structure, GaN nanowires, total energy calculations.

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Corresponding author: H. W. Leite Alves, e-mail: hwlalves@ufsj.edu.br; contact address: Depto. Ciências Naturais (DCNAT), Universidade Federal de São João del Rei, Praça Dom Helvécio, 74, CEP: 36301-160, São João del Rei, MG, Brazil.