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Ab *initio* study of structural and electronic properties of (0001) RuN/GaN short-period superlattices.

C. Ortega López [(1)], R. González Hernández [(2)*], W. López Pérez [(2)] and J. A. Rodríguez Martínez [(3)]

(1) Departamento de Física, Universidad de Cordoba, Montería,Colombia.
(2) GFMC, Departamento de Física, Universidad del Norte, A.A.1569, Barranquilla,Colombia.
(3) GEMA, Departamento de Física, Universidad Nacional de Colombia, A.A. 5997, Bogotá, Colombia.
* rgonzalezh@unal.edu.co

Abstract – We investigate the structural and electronic properties of short-period (1×n) GaN/RuN superlattices (with n≤4) calculated in wurtzite structure with (0001) orientation, using a first-principles calculations within Density Functional Theory (DFT). A detailed studied of the Density of States is made and we have found that the superlattices present metallic behavior. At Fermi level, the Density of States is due to the contributions of d-like-atomic orbitals of Ru. Therefore, the d-Ru orbitals are the responsible of the conduction of charge carriers.

The formation of reliable ohmic contacts to GaN is very crucial for the fabrication of GaN-based electronic and optical devices such as visible light-emitting diodes, high-power microwave devices and metal–semiconductor field-effect transistors. To obtain optimum device performance, the formation of low resistance ohmic contacts to GaN is of great practical importance. In a recent experiment [1] effects on electrical and structural properties of Ru/Au Schottky contact to n-type GaN indicates that the Ru/Au contact could be a useful scheme for the realization of high-temperature device applications. Therefore, it is necessary to study theoretically the electronic structure of Ru/GaN and Au/GaN. Additionally to that fact, we propose to make super lattices of RuN/GaN in wurtzite structure as a possible structure with another interesting physical properties.

In this work, we investigate the structural and electronic properties of short-period (1 × n) GaN/RuN superlattices (with n ≤ 4) calculated in wurtzite structure with (0001) orientation, using a first-principles calculations within Density Functional Theory (DFT). We have employed the Full Potential Linearized Augmented Plane Waves (FP-LAPW) method as implemented in the WIEN2k code [2]. The exchange and correlated effects were treated using the Generalized Gradient Approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [3]. The calculations were carried-out in supercells based on wurtzite structure. In order to determine the best parameters in the wurtzite structure, we have optimized the total energy in function of: (i) the volume of the unit cell, (ii) the relation c/a and (iii) the z-coordinate of Ru and Ga atoms. The 1x1, 1x2, 1x3, 1x4, 2x2, 3x3 and 4x4 superlattices were studied. The volume of the unit cell, the lattice constant and the bulk modulus are showed as a function of the period. A detailed studied of the Density of States is made and we have found that the all super lattices present metallic behavior. At Fermi level, the Density of States is due to the contributions of the d-like-atomic orbitals of Ru. Therefore, the d-Ru orbitals are the responsible of the conduction of charge carriers.

References

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