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Pressure Influence on the Electronic Character of the $Ga_{0.5}Mn_{0.5}N$ Alloy

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Abstract

Computational calculations were performed to investigate the pressure effects on the electronic and magnetic properties of $Ga_{0.5}Mn_{0.5}N$ in the wurtzite structure. The wien2K code was used for carry out the calculations, employing the full-potential linearized augmented plane wave method within the density functional theory. We found that the pressure affects the magnetic properties of alloy because, when the pressure decreases the magnetic moment changes from 0 to 2.85 μ_B at a transition pressure $P_T \sim 24.45$ GPa (and lattice constant of a = 3.156 Å). The value of the magnetic moment increases until reach a constant value of 4.0 μ_B when the pressure decreases towards its equilibrium value (P = 0). Additionally, the density of states study shows that for equilibrium pressure the alloy have a half-metallic behavior, but for a pressure greater than the transition pressure ($P > P_T$) the electronic character of the $Ga_{0.5}Mn_{0.5}N$ change, because the allow acquire the metallic ferromagnetic behavior.

Keywords: Density Functional Theory, pressure effects, electronic and magnetic properties.

INTRODUCTIÓN

The gallium nitride (GaN) is a direct band gap semiconductor material that crystalizes in the wurtzite structure [1-3], The GaN has been extensively studied theorical and experimentally. Due to its superior physical properties GaN have several technological applications, such as: emitters and detectors radiation devices, in high power and high temperature electronics, in blue, green and yellow LEDs, injection lasers and ultraviolet detectors [4-7]. On the other hand, the combination of semiconductor character of the GaN together with the magnetic properties of the transition metals ions such as manganese (Mn), is very interesting to day, due to their potential applications in diluted magnetic semiconductors (DMS). Recently, ferromagnetism at room temperature has been reported theoretical [8-16] and experimentally [17-25]. Ferromagnetism at room temperature is a requirement that must satisfy the material to be a good DMS for potential applications in the spintronic field or as injector spin. In this work, we investigate the pressure effects on the electronic and magnetic properties of $Ga_{0.50}Mn_{0.50}N$ compound.

COMPUTATIONAL METHOD

The computational calculation were performed with Wien2k package [26], using the full-potential linearized augmented-plane-wave method, within density functional theory [27, 28]. The generalized gradient approximation of Perdew, Burke, and Ernzerhof (PBE) [29] was employed to include the interaction effects of exchange and correlations between electrons. In the full-potential linearized augmented-plane-wave method, the cell is divided into two types of regions, the atomic spheres centered at the nuclear sites and the interstitial region between non-overlapping spheres. Inside of the atomic spheres, the wave functions are replaced by atomic functions, whereas in the interstitial region, the function is expanded in plane waves. The charge density and the potentials are expanded in spherical harmonics up to $l_{max} = 10$ inside of the atomic spheres, and the wave function in the interstitial region is expanded in plane waves with a cutoff parameter of $K_{max} = 8/R_{mt}$, where R_{mt} is the smallest radius of the atomic sphere in the unit cell, and K_{max} is the magnitude of the largest *k*-vector of the reciprocal lattice. To ensure convergence in the integration of the first Brillouin zone, 1.600 points were used, which corresponds to 144 *k*-points at the irreducible part of the first Brillouin zone for the wurtzite phase, which obtained with the Monkhorst-Pack method [30]. The integrals over the Brillouin zone are solved using the special approximation of *k*-points of Monkhorst-Pack. For the expansion of the potential in the interstitial region, it is considered that $G_{max} = 12$. The *Muffin-tin* radii were of 1.6 bohr for N, 1.85 bohr for Mn, and 2.0 bohr for Ga. All calculations were carried out with spin polarization, in order to determine the presence of magnetic properties in the compound. The calculation process ended when the forces became smaller than 10^{-4} eV/Å. The convergence threshold for self-consistent field iteration was 10^{-5} eV.

RESULTS AND DISCUSSIONS

Structural properties

First, we reported the results of the calculation of GaN in the structure wurtzite. The equilibrium parameter namely, lattice constant, c/a ratio, bulk modullus, and cohesion energy calculated in this work were: 3.21 Å, 1.639, 191.5 GPa, and -8.96 eV, respectively. All results are excellent agreement with theoretical reports 3.221 Å [31], 1.629 [32], 184.5 GPa [32], and -8.933 eV [31]. The lattice constant and bulk modullus calculated here are in good agreement with the experimental

results 3.19 Å and 188.00 GPa, respectively. The results obtained in this work differ by less than one percent with to respect to theoretical and experimental reported. This smaller percentage show the reliability of our present calculation. For the $Ga_{0.50}Mn_{0.50}N$ compound, we found that crystalize in the hexagonal structure belonging to space group 156 (*P3m1*). To reach $Ga_{0.50}Mn_{0.50}N$ concentration, in the eight atoms supercell we replaced one Ga atom with one Mn atom. The main structural parameters as equilibrium lattice constant, c/a ratio, bulk modullus and, cohesion energy was: 3.19 Å, 1.628, 187.5 GPa, and -8.77 eV, respectively. We note that, as consequence of inclusion of one Mn atom in the matrix of GaN, the lattice constant of $Ga_{0.50}Mn_{0.50}N$ compound decreases. This happen because of atomic radius of Mn (1.26 Å) is smaller than the atomic radius of Ga (1.41 A). In addition, we can see that $Ga_{0.50}Mn_{0.50}N$ compound preserve its rigidity, because the bulk modullus (187.5 GPa) is very close to bulk modullus of the GaN (191.5 GPa).

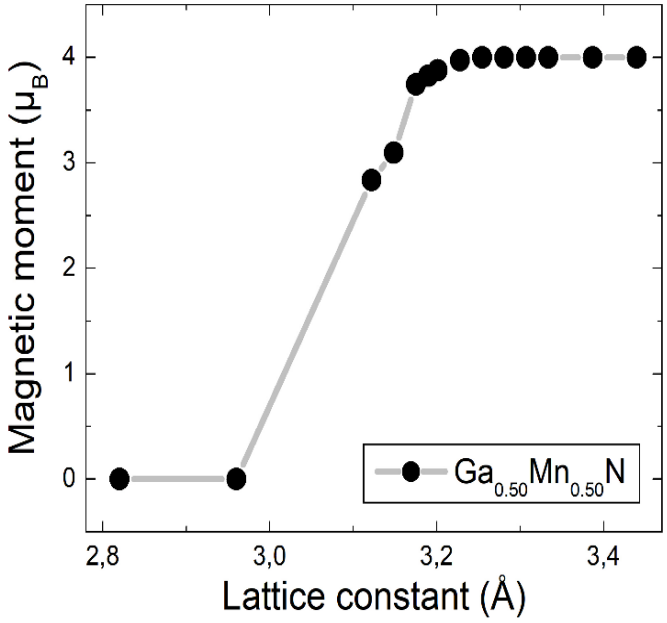

Figure 1. Variation of the magnetic moment as a function of lattice constant for $Ga_{0.50}Mn_{0.50}N$ compound. The points are the calculus and the line is guide to eye. Source: authors.

The figure 1 shows the variation of the magnetic moment as a function of the lattice constant. We found that the magnetic moment changes from 0 to 2.85 μ_B, with lattice constant of 3.156 Å, corresponding at transition pressure of P_T = 24.45 GPa. This result indicates that magnetic properties change with the pressure and therefore, can be manipulated experimentally. In the figure 1, we note that the magnetic moment increases until reach a constant value of 4.0 μ_B/cell, when lattice constant increase to its equilibrium value, or other words, when the pressure decreases towards its equilibrium value (P = 0).

Electronic Properties

To analyzes the pressure influence on the electronic properties of $Ga_{0.50}Mn_{0.50}N$ compound first calculated the density of state at the equilibrium pressure, and before at a pressure higher than the transition pressure ($P > P_T$).

Figure 2 shows the total and partial density of states calculated with the equilibrium lattice constant (therefore at equilibrium pressure P = 0). It can be observed that, near the Fermi level, the $Ga_{0.50}Mn_{0.50}N$ compound becomes conductor for the spin-up density. This is mainly determined by the Mn-3d states and to a lesser extent, by the N-2p electrons. On the other hand, the compound becomes a semiconductor for spin-down density (no spin-down contribution). Therefore, the compound exhibits a half-metallic ferromagnetic behavior at P = 0. This compound have 100% spin polarization of the conduction carriers and satisfy the first requirement to be a good diluted semiconductor material, with potential application in spintronic or as spin injectors.

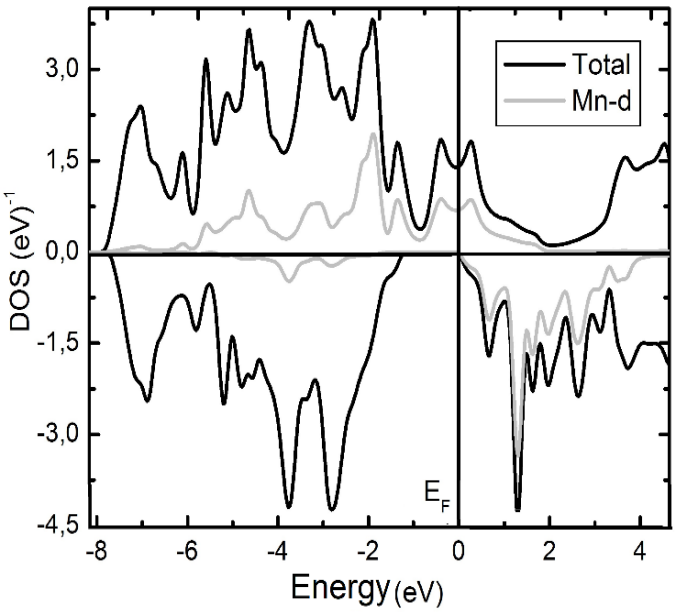

Figure 3. Total and partial density of state for $Ga_{0.50}Mn_{0.50}N$ compound in the wurtzite structure at equilibrium pressure P = 0. Source: Authors.

The figure 3 shows the total and partial density of states of $Ga_{0.50}Mn_{0.50}N$ compound calculated at high pressure (namely P = 30 GPa, which exceeds the transition pressure, $P > P_T$ = 24.45 GPa). In both, the valence and conduction band, there are spin-up and spin-down polarization. Additionally, due to the effect of pressure, the superlattice loses its half-metallic character, because the two spin channels (spin-up and spin-down) crosses the Fermi Level, the compound has a metallic behavior. In this case, the compound has magnetic properties because the spin up and spin down are not symmetrical. The compound has a magnetic moment with a value of 2.85 μ_B.

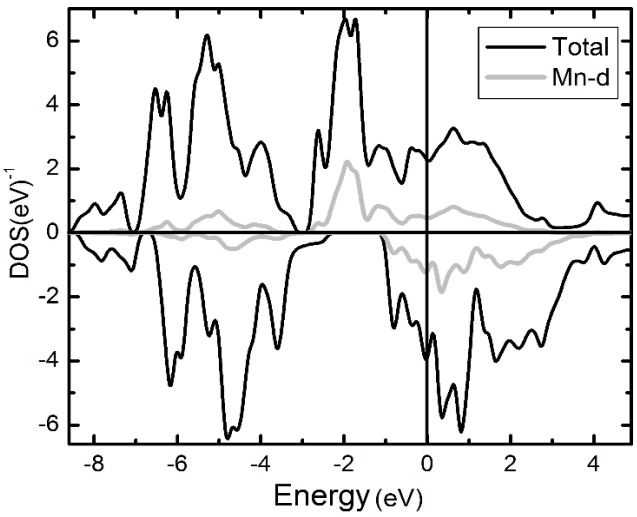

Figure 3. Total and partial density of state for $Ga_{0.50}Mn_{0.50}N$ compound in the wurtzite structure calculated at high pressure ($P > P_T = 24.45$ GPa) in this case P = 30 GPa. Source: Authors

CONCLUSIONS

In this work, we reported the results of the study of pressure influence on the electronic and magnetic properties of $Ga_{0.50}Mn_{0.50}N$ compound. The calculation were performed in the wurtzite structure in the framework density functional theory, employing the full-potential linearized plane wave method and using the computational Wien2k code. The analyses of the magnetic moment as a function of the pressure shows that the magnetic moment changes for a transition pressure P_T; in particular, we found that the magnetic moment changes from 0 to 2.85 μ_β at a transition pressure of $P_T \sim 24.45$ GPa. On the other hand, the study of the density of states reveal that at equilibrium pressure P = 0 GPa the compound has half-metallic ferromagnetic behavior with a magnetic moment of 4.0 μ_β/cell. The magnetic properties come from of the polarization of the Mn-3d states mainly. The density states shows that for to high pressure ($P > P_T = 24.45$ GPa). For the case P = 30 GPa, the electronic behavior of the compound change, because the compound has a metallic behavior. The result shows that the spin polarization is dependent on pressure and may be manipulated experimentally.

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