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SEMI-METAL FERROMAGNETISM V-DOPED GaN NANOSHEET APPLICATION IN A SPINTRONIC DEVICE

The density functional theory calculations using general gradient approximation (GGA) have been systematically performed to study the electronic structures, the density of states (DOS), and magnetic properties of V-doped GaN nanosheet for different dopant concentrations (2.08% and 4.16%). We conducted the entire study using the Atomistix ToolKit code. The electronic properties were improved with the Hubbard values U = 4 eV. V-doped CaN nanosheet exhibits stable ferromagnetic (FM) states relative to corresponding antiferromagnetic (AFM) states. The calculated TC with the V-doping is found to be above the room temperature (RT) one. Calculation results reveal that V-doped nanosheets may be good candidates for spintronics due to their good half-metal ferromagnetism.

K e y w o r d s: DFT, approximation, magnetic moment, nanoribbon.

1. Introduction

Nowadays, semiconductors doped with different transition metals have been considered the most promising room temperature-diluted magnetic semiconductor (DMS) materials [1, 2] which are considered very interesting topics in the materials science community due to their high potential applications in spintronics [3, 4].

For example, GaN, which has a wide bandgap of 3.4 eV, has been studied both experimentally and theoretically. Doping of semiconductor nanocrystals (NCs) with transition metal ions has attracted significant interest in applications such as blue light-emitting diodes, room-temperature laser diode, optical coating, solar cells, and especially photovoltaic devices [5, 6]. Nanosheet, nanoribbon, and monolayer structures of GaN are well-known as non-magnetic semiconductor materials [7–10].

Among works devoted to the investigation of TM doped GaN nanosheet, monolayer, and nanotube are reported the room temperature ferromagnetism for (Ga, Mn)N [11], (Ga,Cr)N [12], (Ga,Cu)N [13], (GaMn)N [14]. Pristine GaN monolayer is a wide-gap semiconductor, whereas Mn-doped GaN monolayer becomes p-type and n-type semiconductors depending on the site of doping. Such properties lead to its use in opto and nanoelectronics applications [15]. Substituting a cation Ga atom with TM leads to a structural distortion around $3d$ TM impurity in the GaN nanosheet [16]. For Cr-, Mn-, Ni-doped GaN nanosheet FM ordering and Fe-doped GaN nanosheet AFM ordering are more favorable.

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A half-metallic ferromagnet, in which a completely spin-polarized current is expected, is considered an optimal candidate for spintronic devices.

Calculation of electronic and optical properties of 12.5% V-doped GaN crystal structure using the first-principles method based on the density functional theory, shows that the ferromagnetic state is stable and curie temperature is found to be above the room temperature. The analysis of optical properties shows that V-doped GaN is a promising dielectric material and has potential applications in optoelectronic devices [16].

In this article, electronic, optical and magnetic properties of V-doped (2.08% and 4.16%) GaN nanosheets have been investigated. Inspired by the above similar discussed materials. We explored the GaN nanosheet doped with various concentrations of V atoms, since among the listed works electronic and magnetic properties of V-doped GaN nanosheet are absent. The outcomes suggest the use of these compounds for optoelectronic devices.

2. Computational Method

Our calculation was performed using the Atomistix ToolKit (ATK) program package based on density-functional theory (DFT). The SG15 functional coupled with the generalized gradient approximation (GGA) was used for the exchange-correlation potentials. Monkhorst–Packgrid of $1 \times 1 \times 15$ is used for structure optimization and a $1 \times 1 \times 20$ mesh for the electronic-structure calculations. The real space grid for a GaN nanosheet, is calculated with mesh cut off energy of 150 Ry and a double-zeta polarization (DZP) basis set for all of the atoms to achieve the balance between the calculation efficiency and accuracy. As mentioned in other DFT studies, GGA does n't account for the localization of d or f orbitals of transition metals. To include the effects of localization of the d-state of V, the GGA $+ U$ method is employed. The value $U = 4$ eV for $3d$ state is from prior literature. A vacuum region of about 10 Å along the nonperiodic directions is employed to avoid any interactions between adjacent supercells. In all the calculations, the atomic coordinates are relaxed until the Hellman–Feynman forces are below 0.01 eV A^{-1} and the total energy changes are less than 10^{-3} eV. The spin polarization scheme has been carried out to investigate 2.08% and 4.16% V-doped GaN nanosheets which are consistent from 96 atoms.

3. Results

To investigate the electronic properties at the first step, the electronic band structures for pure GaN nanosheet (Fig. 1) are calculated. As can be seen from Fig. 1, *d*, the band gap equal to 2.76 eV of pure GaNNS, is narrow in comparison to bulk GaN [17–19]. But it is higher than previous theoretical calculations for GaN nanosheet to be 1.76 eV [8], 1.95 eV [20]. It should be noted that we have several works [22–26], where different methods were used to correct the band gap for various compounds and, in the presented work, GGA-SG15-Hubbard U combination gives the best result. Taking into account that the main goal of this work is not to compare different pseudopotential results, we will conduct further calculations with GGA-SG15-Hubbard U combination without showing other results.

In the presented of spin-polarized DOS calculation (Fig. 1, *c*) completely symmetrical spin-up and spin-down indicate that the pure structure of GaNNS is a nonmagnetic semiconductor. These results are consistent with previous studies [8, 25, 26]. From Fig. 1, *c*, we can see that a vicinity of the Fermi level is associated with the $2p$ orbitals of N and the $4s$ orbitals of Ga atoms. For investigation of electronic and magnetic properties of V-doped GaNNS, Ga atoms were replaced by V atoms at various 2.08%, 4.16%, and 8.3% concentrations. As reported in Refs. [27, 28], TM atoms prefer to be doped on the Ga site. Thus, in this work, we directly employed the Ga site for the V-doping.

Optimized bond lengths between the V atom and its nearest-neighbor N atoms is 1.84 Å. The difference in bond lengths from the pure Ga–N bond lengths 1.86 Å due to the different ionic radii of V atom. The total energy and magnetic moment of the nanosheet for each of three different concentrations (2.08%, 4.16%, and 8.31%) of V atoms, the relative energies between FM and AFM states and magnetic moments are listed in Table. A positive ΔE value means that the FM state is energetically more stable for a V-doped nanosheet.

From electronic structure analyses Figs 2 and 3, it is clear that the V atom induces an intermediate band between the VB and the CB in the spin-up state, which intersects the intermediate band and makes makes a partially filled band. Depending on the V concentration, the width of the impurity band

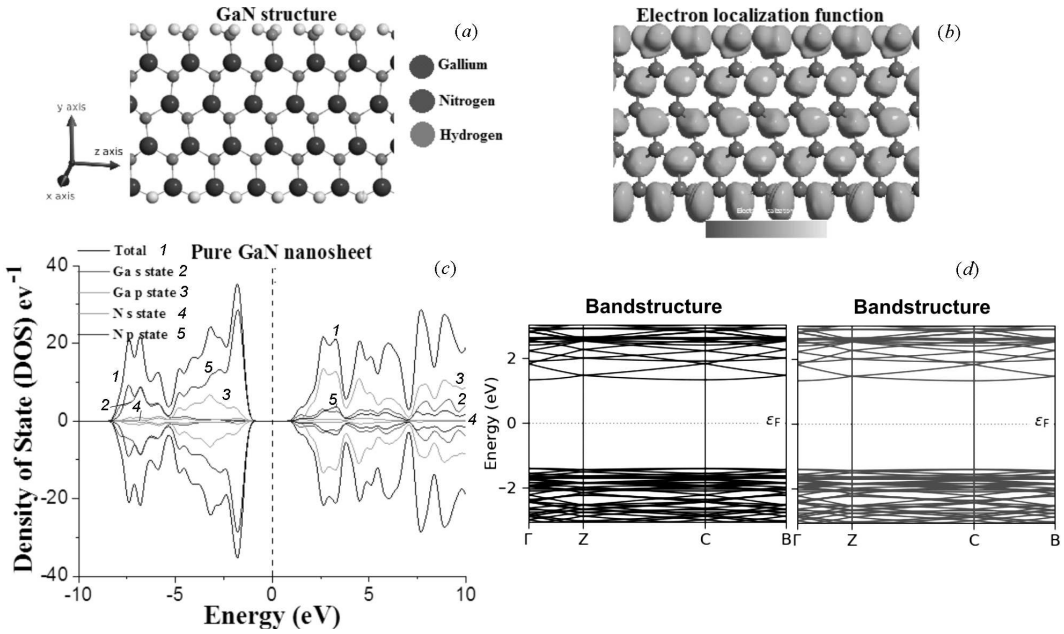


Fig. 1. The optimized structure of (*a*) the nanoribbon GaN with 96 atoms (*a*), electron localization function (*b*), the total and partial density of states (*c*), the colored lines represent the contribution of different orbitals in the DOS, the Fermi level is set at zero energy and is indicated by a vertical dashed line, calculated band structure for spin up (black) and spin down (red) (*d*) Fermi level is set at zero energy and is indicated by a horizontal dashed line

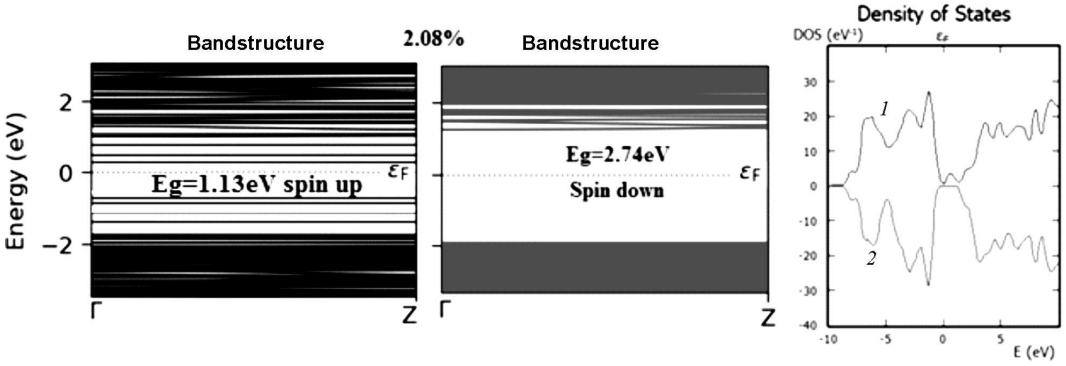
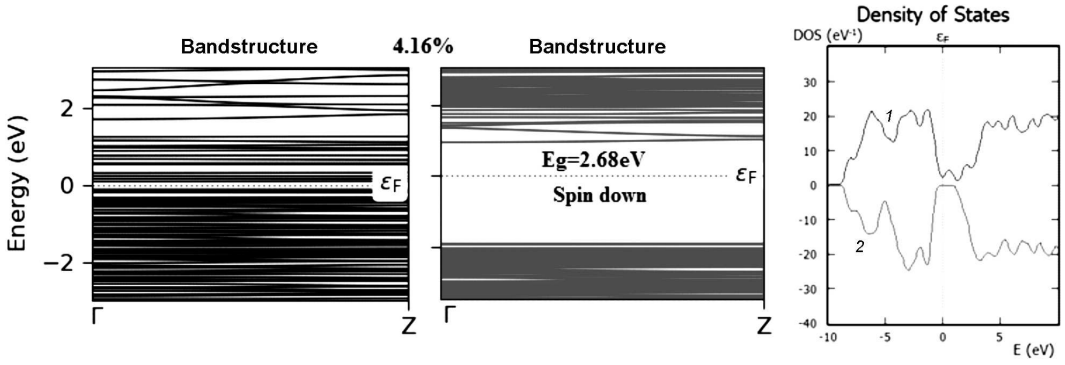


Fig. 2. Spin-resolved band structure and total DOS for vanadium doped (concentration 2.08%) GaN nanosheet. The black and red band structure shows spin-up (*a*) and spin-down bands respectively (*b*) and the right hand shows the total DOS (*c*). The Fermi level is indicated by a dashed line

Total energy of FM, AFM states, magnetic moments and Curie temperature T_C of doped with different concentration V–GaN nanosheet

Concen. %	E_{FM} (eV)	E_{AFM} (eV)	ΔE	Magnetic moments (μ_B)	T_C (K)
2.08	–67247.28057	–67247.26547	–0.0151	4.58	302
4.16	–67247.66777	–67247.65482	–0.01297	9.16	214



a *b* *c*

Fig. 3. Spin-resolved band structure and total DOS for vanadium-doped (concentration 4.16%) GaN nanosheet. The black and red band structure shows spin-up (*a*) and spin-down bands (*b*) respectively and the right hand shows the total DOS (*c*). The Fermi level is indicated by a dashed line

increases gradually the value of spin up and spin down gap are: for 2.08% spin up-1.13 eV and spin down-2.74; for 4.16% spin up-0, and spin down-2.68.

As can be seen from the Figs. 2 and 3, conduction band spin polarization is more obvious, where the spin-up band occupies the Fermi level, while the spin-down band does not occupy the Fermi surface (2.08%). At the bottom of the conduction band, in the spin-up band 3*d* state of V and 2*p* state of N are strong hybridization. In the 4.16% concentration of V atom valence and conduction bands overlap with each other for the spin-up states, while, for spin-down states, there is still a wide band gap. As explained in Ref. [16], the observed half-metallic ferromagnetism properties can be explained within the framework of crystal field theory. Observed ferromagnetism for V-doped GaNNS is in a good agreement with results obtained for GaN bulk [7, 29] and nanostructures [30].

Mulliken analysis shows that the introduction of the V impurity (2.08%) induces a total magnetic moment of 4.58 μ_B. The magnetic moments on per V and adjacent N and Ga atoms were 2.21 μ_B, 0.07 μ_B and 0.002 μ_B, respectively. Contribution to the magnetic moment is mainly from highly spin-polarized V atom. The slightly high value of magnetic moment on the neighboring N atom compared to Ga atom is related to strong hybridization between N-*p* and V-*d* orbitals. For 4.16% concentration of V, magnetic moments per V and N and Ga atoms were 0.002 μ_B, respectively. The Curie temperature (Tc) was evaluated by using the mean-field approximation for various concentrations of V atoms. Taking into account that the energy difference $E_{FM} - E_{AFM} = -0.0151$ (2.08%) and –0.02297 (4.16%), *Tc* is determined as 302 K and 214 K, respectively. Thus, doped with a low concentration of V, the GaN nanosheet can be considered a promising material for practical applications.

4. Conclusions

In conclusion, a V-doped GaN nanosheet with V concentrations 2.08% and 4.16% was investigated within GGA-SG15-Hubbard *U* method. We have shown that substituting V atoms at cation (Ga) sites can significantly modulate the magnetic properties of nanosheets, transforming it into a half-metallic ferromagnet. Obtained from Mulliken analyses total magnetic moments are 4,58 and 9.16 for 2.08% and 4.16% concentration of V atoms. The main contribution to the magnetization is from the *d*-states of V atoms. The Curie temperature, above room temperature, is an interesting discovery for special applications in spintronics devices.

The data that support the findings of this study are available from the corresponding authors upon reasonable request.

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ФЕРОМАГНЕТИЗМ НАПІВМЕТАЛЕВИХ НАНОЛИСТІВ GaN, ЛЕГОВАНИХ ВАНАДІЄМ, ТА ЙОГО ЗАСТОСУВАННЯ У СПІНТРОННИХ ПРИСТРОЯХ

Проведено розрахунки в рамках теорії функціонала густини та з використанням узагальненого градієнтного наближення для вивчення електронних структур, густини станів і магнітних властивостей GaN нанолистів, легованих атомами ванадію (V-GaN-НЛ), з різними концентраціями легуючих домішок (2,08% і 4,16%). Всі розрахунки проводилися за допомогою програмного пакету Atomistix ToolKit. Виявлено покращення електронних властивостей V-GaN-НЛ при значенні параметра Хаббарда $U = 4$ еВ. V-GaN-НЛ демонструють наявність стабільних феромагнітних станів відносно відповідних антиферомагнітних станів. Виявлено, що розраховане значення температури Кюрі для V-GaN-НЛ перевищує кімнатну температуру. Результати розрахунків показують, що V-GaN-НЛ можуть бути гарними кандидатами для спінтроніки завдяки їхнім проявам феромагнетизму.

Ключові слова: теорія функціонала густини, апроксимація, магнітний момент, нанострічка.