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First principles study of the electronic structures and magnetic properties of transition metal-doped cubic indium nitride

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ABSTRACT

First principles density functional calculations, using a full potential linearized augmented plane wave (FP-LAPW) method in local spin density approximation(LSDA), have been performed in order to investigate the structural, electronic and magnetic properties of $In_{1-x}TM_xN$(TM=Cr,Fe,Mn,V) in zinc-blende phase. Dependence of structural parameter values on the composition x have been analyzed in the $x=0.25$, $x=0.50$, and $x=0.75$, we found the existence of deviation from Vegard's law. Calculated electronic structure and the density of states of these alloys are discussed in terms of the contribution of TM 3d, N 2p, and In 3d states. The magnetic moment of $In_{1-x}TM_xN$ has been studied by increasing the concentration of TM atom. The contribution of TM atom is the most important source of the total magnetic moment in these alloys, while it is minor in In and N.

1. Introduction

Group-III nitride semiconductors have attracted great attention over the past decade due to its intriguing optoelectronic properties and high thermal and mechanical stability [1]. These semiconductors are now widely used in efficient short-wavelength (blue and ultraviolet) light-emitting diodes (LEDs), room temperature laser diodes and field-effect transistors [1]. The diluted magnetic semiconductors (DMSs), which have both ferromagnetic and semiconducting properties, are a unique type of promising materials for the fast emerging field of spintronics. The DMSs are created by doping the magnetic ions like Cr, Mn, Fe, and Ni, into a semiconducting host such as GaAs, GaN, ZnO and ZnTe [2–4], a great effort has been focused on these materials both experimentally and theoretically. For systematic studies, it includes the structural, electronic and magnetic properties for 3d transition metal by using a linear muffin-tin orbital (LMTO) method both in the rocksalt (NaCl) and zinc-blende structures [5]. Furdyna [6] shows the exchange interaction between the spin of s, p electrons of host with the d electrons of the doped transition metal ions which are responsible for magnetic, optical and conductive properties of DMS materials.

Gallium nitride (GaN) and aluminum nitride (AlN) are two of the most promising III–V semiconductors for short wavelength optoelectronic devices. InN has received the same attention as GaN and AlN primarily because the 1.9 eV band gap for InN corresponds to a portion of the electromagnetic spectrum in which an alternative semiconductor technology exists. The band gap of this material is direct; indium nitride crystallizes as a hexagonal wurtzite structure under normal conditions [7–9], and its successful growth [10] has also reported that InN grows in zinc blende structure. Serrano et al. [11] confirmed that the ZB phase is indeed metastable using first-principles calculations. The success of the commercialized InGaN alloys [12,13] of Nichia Chemical Industries as light emitting diodes and laser diodes has drawn the attention of the scientific community to the validity of the presumed band

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gap of ~1.9 eV of InN [14]. Recently it has been reported that InN exhibits a narrow direct band gap energy of around 0.7 eV [15,16], which means that by modulating the concentration of indium in the $In_xGa_{1-x}N$ alloys, a wide spectral range from infrared to ultraviolet can be obtained.

2. Computational details

The calculations were performed using a scalar relativistic FP-LAPW method within density functional theory (DFT)) implemented in the WIEN2K code [17] to study the local magnetic structures around substitutional TM (V, Cr, Mn, Fe) impurities doped at cation sites in ZB structures of InN. For the exchange and correlation potential, we use the local spin density approximation (LSDA) [18]. A mesh of 64 special k-points is taken in the whole Brillouin zone, we use a parameter $R_{MT}K_{max}=$ 8, where K_{max} is the plane wave cut-off and R_{MT} the smallest of all atomic sphere radii, while the charge density was Fourier expanded up to $G_{max}=14$ Bohr^{-1}, where G_{max} is the largest vector in the Fourier expansion. The calculated total energies were applied to the Murnaghan equation of state [19] to obtain the energy–volume relation and hence the bulk modulus. The R_{MT} values for InN are assumed to be 2.10 and 1.65 a.u. for In and N, respectively. The electronic configuration for InN is In:Kr $4d^{10}5s^25p^1$, N:He $2s^22p^3$, and the electronic configuration of TM are V:Ar $4s^2$ $3d^3$,Cr: Ar $4s^1$ $3d^5$ Mn:Ar $4s^2$ $3d^5$, and Fe: Ar $4s^2$ $3d^6$. For the electronic configuration of TM ions we use: V^{3+}: Ar $3d^2$(with 2 electrons at eg state), Cr^{+3}: Ar $3d^3$(with 2 electrons at eg state and 1 electron at t2g state), Mn^{+3}:Ar $3d^4$(with 2 electrons at eg and 2 electrons at t2g state) and Fe^{+3}:Ar $3d^5$(with 2 electrons at eg state and 3 electrons at t2g state).

3. Results and discussions

3.1. Structural properties

Before calculating the electronic structure and magnetic properties, volume optimization of $In_{1-x}TM_xN$(TM= Cr, V, Mn, Fe) has been performed. The values of lattice constant '*a*', bulk modulus *B*, determined by fitting the total energy as a function of volume using the Murnaghan's equation of state [19].

$$E(V)=E_0(V)+\frac{BV}{B'(B'-1)}\left[B\left(1-\frac{V_0}{V}\right)+\left(\frac{V_0}{V}\right)^{B'}-1\right] \quad (1)$$

The lattice constant *a*, the bulk modulus *B* and first order pressure derivative of the bulk modulus *B*', for

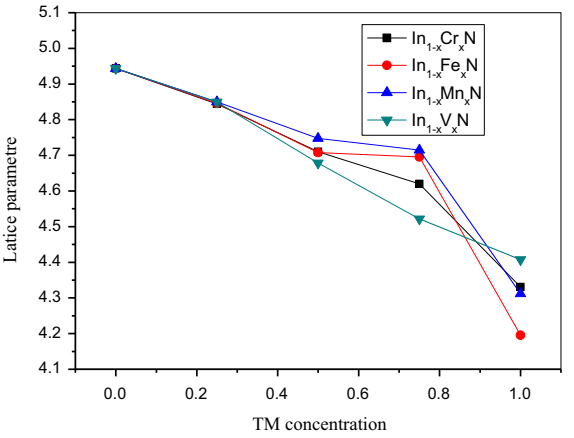

Fig. 1. Calculated lattice constant as a function of TM composition.

Table 1
Calculated lattice constants '*a*', bulk modulo *B* and the first order pressure derivative of the bulk modulus, B_0 for different concentrations of TM

Compound	*x*	*a* [Å]	*B* [GPa]	B_0 [GPa]
$In_{1-x}Cr_xN$	0.00	4.9438	146.4532	4.8700
		4.94[20]	146[20]	4.48[20]
	0.25	4.8441	160.8867	5.3627
	0.50	4.71	171.52	4.6286
	0.75	4.62	281.78	8.400
	1	4.3309	332.7275	7.9803
$In_{1-x}Fe_xN$	0.00	4.9438	146.4532	4.8700
	0.25	4.8460	160.5806	5.3554
		4.812[21]	156.45[21]	4.55[21]
	0.50	4.7078	148.5549	4.4155
	0.75	4.6953	409.5474	13.9728
	1	4.1955	436.4316	7.8518
$In_{1-x}Mn_xN$	0.00	4.9438	146.4532	4.8700
	0.25	4.8499	158.1901	5.4632
		4.815 [21]	157.72 [21]	4.22 [21]
	0.50	4.7474	176.4365	5.8330
	0.75	4.7150	306.5079	10.4838
	1	4.3118	1290.4286	34.2606
$In_{1-x}V_xN$	0.00	4.9438	146.4532	4.8700
	0.25	4.8496	164.5173	5.2738
	0.50	4.6782	328.7212	5.3670
	0.75	4.5014	190.8131	9.3028
	1	4.4676	221.7884	7.3912