Investigation on half-metallic ferromagnetism in Phosphorous doped SmN- Band structure study

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Abstract. Rare earth nitrides with electronic and magnetic properties would be advantages for the development of spintronic devices. Structural, electronic, magnetic and elastic properties of rare earth nitrides namely SmN and SmN0.5P0.5 compounds are studied by using the spin-polarized full potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT). A supercell scheme is used to carry out the ground state calculations of SmN0.5P0.5. The structural parameters, band structure, density of states and charge densities have been analysed by generalized gradient approximation (GGA) for ferromagnetic phase and the results are verified by using charge density plots.

1. Introduction
De Groot et al [1] have introduced the half-metallic ferromagnetism concept, with band structure calculations in semi Heusler compounds. Half metals are very strong ferromagnets. From this unusual property, compounds are metal for one spin state and semiconductors or insulators or semimetals for the opposite spin state. In half metals, at the Fermi level the spin polarization of electrons is 100% at the Fermi level, which is the required condition for spintronics applications and also used as spin transistor, as defined by M. Johnson [2]. SmN has wide applications in spintronic devices. The study of band structure is of huge importance in studying compound materials to understand their physical properties. The fascinating physical properties and new technological applications of half-metals in spintronics devices have more attention in the past decade [3].

To make spintronic devices, the diluted magnetic semiconductors (DMS) are one of the important materials [4]. The necessary condition for making spintronic devices is the diluted magnetic semiconducting materials can be characterised as exact half metallic ferromagnets and at the Fermi level with 100% spin polarization. Magnetic characteristics of SmN have been reported by Schumacher et al and Busch et al [5-6]. Didchenko et al. studied electric and magnetic properties of SmN [7]. Preston et al [8] compared SmN with DyN experimentally and theoretically. Hence, computational details for the physical properties of phosphorus doped SmN with x=0.5 doping concentration has been reported.

2. Computational Details
Calculations were performed using programming package Wien2k [9], which is a full potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT) [10]. Density functional theory has proved to be an important tool for studying properties of metals, semimetals, semiconductors, half-metals etc., Exchange correlation terms are treated by the Perdew-Berke-
Ernzerhof (PBE) [11]–generalized gradient approximation (GGA) [12]. For the Brillouin-zone integration, the 10 x 10 x 10 Monkhorst-pack mesh is used. The basis sets are fixed with $R_{MT} \times K_{max} = 7$, $l_{max} = 10$ and $G_{max} = 12$. The convergence criterion is fixed to 0.0001 Ry for energy and 0.001e for charge. The muffin-tin radius of samarium and nitrogen are assumed as 2.4 and 2.12 respectively. For making SmN$_{0.5}$P$_{0.5}$, 2x2x2 supercell has been created and 4 nitrogen atoms are replaced by 4 phosphorous atoms.

3. Result and Discussions

3.1. Structural properties

SmN belongs to rock salt NaCl structure with the space group Fm-3m and space group number 225. Samarium and Nitrogen atom is located at (0.5,0.5,0.5) and (0,0,0) respectively. Birch-Murnaghan equation of state [13] is used to determine the ground state properties. Fig. 1a&1b shows that the X-crysden [14] plots of (001) plane of cubic SmN and SmN$_{0.5}$P$_{0.5}$.

Table 1 gives the spin-generalized gradient approximation calculated lattice constant $a_{opt}$, bulk modulus(B), pressure derivative (B’), total energy ($E_{tot}$), Fermi energy ($E_F$) of both spin-up and down states and Magnetic moment ($\mu_B$). The calculated results of SmN and SmN$_{0.5}$P$_{0.5}$ for ferromagnetic (FM) phase are agreed well with available experimental and theoretical work.

|          | SmN | SmN$_{0.5}$P$_{0.5}$ |
|----------|-----|----------------------|
| $a_{opt}$ (Å) |     |                      |
| B (GPa)   |     |                      |
| B’        |     |                      |
| $E_{tot}$ (eV/atom) |     |                      |
| $E_F$ (eV) |     |                      |
| $\mu_B$ (μB) |     |                      |

Table 1. Calculated $a$(Å$^0$), bulk modulus $B$(GPa), pressure derivatives($B’$), Fermi energy ($E_F$) and Magnetic moment ($\mu_B$) of SmN and SmN$_{0.5}$P$_{0.5}$ for spin-up and spin-down channel.
### Compounds Calculations

| Compounds            | Calculations | $a_0$(Å) | B(GPa) | $B'$ | $E_F$ | $\mu_B$ |
|----------------------|--------------|----------|--------|------|-------|---------|
| Exp                  |              | 5.0432   |        |      | 0.6145↑ |         |
| SmN                  | This work    | 5.0388   | 126.9173 | 4.3367 | 0.6145↓ | 4.99    |
| SmN$_{0.5}$P$_{0.5}$ | This work    | 11.0004  | 76.8977 | 4.3080 | 0.5114↑ | 40      |

#### 3.2. Electronic properties

**3.2.1. Band structure.** The ferromagnetic electronic band structures of SmN and SmN$_{0.5}$P$_{0.5}$ are plotted with high symmetry Brillouin zone (BZ) and presented in Fig 2a&2b. From the band structure, it is observed that the metallic behavior of majority spin and the clear visible band gap of minority spin coexist at Fermi level for both SmN and SmN$_{0.5}$P$_{0.5}$. It is clearly visible that SmN and SmN$_{0.5}$P$_{0.5}$ are half metal. The bands at the fermi level is mainly due to Sm-f states and at the same hybridization between Sm f- states and N p-states can also be seen; the bands below the Fermi level is due to N p-states and a minor contribution from Sm p- and d- states; and the bands above the Fermi level is mainly due to Sm d- states and also there is a little contribution from N and P p- states. Spin magnetic moment occurs because of splitting of Sm 4f majority and minority spin. In Fig.(2b), the lowest energy bands in valence band are due to N and P p- states. In Fig. (2b & 3b), the Sm f- states is shifted to the conduction band. The bottom of the conduction band and top of the valence band meet at the X point (Fig.2b) in the Brillouin zone for SmN, whereas for SmN$_{0.5}$P$_{0.5}$, it has been meet at Γ point (Fig.3b). A considerable half metallic gap of 0.65 eV and 0.5 eV is found in SmN and SmN$_{0.5}$P$_{0.5}$ respectively that is approachable for spin conduction.

![Figure 2a. Band structure of SmN spin-up channel. Figure 2b. Band structure of SmN spin-down channel.](image)

3.2.2. Density of states. The total and partial density of states [15] of SmN₀.₅P₀.₅ for both spin channels are shown in Fig. 4a & 4b. The high peak of the strongly localized Sm-4f states is separable from other states of the DOS in SmN₀.₅P₀.₅. This hybridization reflects in the total magnetic moment and localized Sm-4f states responsible for magnetic properties. The total magnetic moment (μB) of SmN and SmN₀.₅P₀.₅ are equal to 4.99 μB and 40μB which confirmed the half metallic behavior.
3.2.3. Charge Density Plot. The charge densities of P doped SmN with concentration 0.5 in the plane (001) is analyzed using GGA as shown in fig 5a&5b. From the figure, it is clearly observed that the spherical contours around the vicinity of Sm- and N- atom as evident for metallic bonding nature of SmN. In Fig. 5b, it is found that the directional charge density contours enclosed Sm - P - Sm atoms in SmN0.5P0.5 indicates the covalent nature of the material.

![Figure 5a. Spin polarized charge density plots of SmN.](image_url)
![Figure 5b. Spin polarized charge density plots of SmN0.5P0.5.](image_url)

3.3. Elastic Properties

Elastic constants C_{11}, C_{12} and C_{44} are calculated for SmN and SmN_{0.5}P_{0.5} at ambient condition by using Thomos Charpin method [16]. Mechanical properties such as Young’s modulus, Bulk modulus, Shear modulus, Cauchy’s pressure [17], G/B ratio, Poisson’s ratio and hardness values are calculated by using three cubic elastic constants C_{11}, C_{12} and C_{44}. The calculated values are represented in Table 2. According to mechanical stability criteria [18,19], the SmN and SmN_{0.5}P_{0.5} has to be confirmed that mechanically stable. Ductile/Brittle nature of the material has been analysed by using the mechanical properties calculated by the elastic constants. Poisson ratio shows that the SmN and SmN_{0.5}P_{0.5} are in ductile nature. Hardness value indicates that the SmN is less hard material and SmN_{0.5}P_{0.5} is a hard material when compared to SmN.

| Parameters         | SmN   | SmN_{0.5}P_{0.5} |
|--------------------|-------|------------------|
| C_{11}(GPa)        | 134.0295 | -26.0406       |
| C_{12}(GPa)        | 57.088 | 31.5317         |
| C_{44}(GPa)        | 92.779 | 19.7806         |
| G(GPa)             | 35.735 | 31.2659         |
| E(GPa)             | 93.7156 | 50.8507        |
| C_{12}-C_{44}(GPa) | 41.251 | 11.751          |
| G/B                | 0.4   | 2.5             |
| v                  | 0.31  | 0.1867          |
| H_v                | 3.435 | 29.83           |

![Table 2. Calculated elastic properties of SmN and SmN_{0.5}P_{0.5.}](image_url)
4. Conclusions

First principles calculations of structural, electronic, magnetic and elastic properties of cubic binary SmN and ternary SmN$_{0.5}$P$_{0.5}$ have been performed by using DFT approach. From band structure calculation it is found that the half metallicity exists in both SmN and SmN$_{0.5}$P$_{0.5}$ materials for ferromagnetic phase. The P-doped SmN is identified as half metallic ferromagnets with 100% spin polarization at $E_F$. Half metallic gap at $E_F$ is due to the shifting of Sm 4f- states to the conduction band (above the Fermi level) and also hybridization between Sm 4f- and P 3p- states. The Sm 4f- states contributes more due to total magnetic moment and N/P atoms have minor contributions. The presence of half metallicity in SmN and SmN$_{0.5}$P$_{0.5}$ creates it probable material for spintronic applications.

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References

[1] De Groot R A et al 1983 Phys. Rev. Lett. 50 2024-2027
[2] Johnson M 1995 J. Magn. Mater 140 21
[3] Amin B et al 2011 J. Electron. Mater 40 6
[4] Zitouni A et al 2014 J.Solid State Commun 190 40-43
[5] Schumacher D P and Wallace W E 1966 Inorg. Chem. 5 1563
[6] Busch G et al 1965 Phys. Lett. 14 264
[7] Didchenko R and Gortsema F P 1963 J. Phys. Chem. Solids 24 863
[8] Preston A R H et al 2007 Phys. Rev. B 76 245120
[9] Blaha P et al 2001 WIEN2k: an augment plane wave plus local orbitals program for calculating crystal properties (Wien, Austria: \K Schwarz Technical University)
[10] Kohn W and Sham L J 1965 Phys. Rev. 140 A1133
[11] Perdew J P et al 1966 Phys. Rev. Lett. 77 386
[12] Perdew J P et al 1992 Phys. Rev. B 46 6671
[13] Murnaghan F D 1947 Proc. Natl. Acad. Sci.USA 30 244
[14] Kokalj A 2003 Comput. Mater. Sci. 28 155
[15] Manjula M et al 2016 Mater. Chem. Phys 181 1-9
[16] Jamal M, 2012 Cubic-Elastic, http://www.wien2kat/reg_user/unsupported/cubic-elast/2012
[17] Pettifor D 1992 Mater. Sci. Technol 8 345
[18] Shi D et al 2009 J. Solid State Chem. 182 2664
[19] Manjula M and Sundareswari M 2016 Materials Today: Proceedings 3 2991–2996