

The electronic band structure of Nd₂Fe₁₄B from First-Principles calculations

Abeer E. Aly

Basic Science Department, Modern Academy for Computer Science and Management Technology, Cairo, Egypt.

Abstract- Electronic structure calculations for the permanent magnet material Nd₂Fe₁₄B has been calculated using spin-polarized full potential linearized augmented plane wave (FPLAPW) method. This method is highly effective for systems with very complex structures. The results presented include the band structure of Nd(4f) site and their partial density of states (DOS). The band structure for Nd (4f) site is in good agreement with the self-consistent calculations. We calculated the results for Nd₂Fe₁₄B by spin polarized without spin-orbit coupling.

Correspondence Author – (abeerresmat782000@yahoo.com)

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1. INTRODUCTION

Nd₂Fe₁₄B is the most important materials in the series in terms of practical applications and is the one most intensively studied [1]. Some empirical and non-self consistent calculations have been reported on the electronic structure of Nd₂Fe₁₄B [2-8]. We study the density functional theory (DFT) using self-consistent full potential linearized augmented lane wave (FPLAPW) method [9]. The potential Linearized Augmented Plane Wave and the electron density are separated into two regions, i.e. in the non-overlapping atomic spheres (region I) and the interstitial regions (region II). The wave function solutions of the Kohn-Sham equation are expanded in augmented wave functions. In region I, they are expanded in radial functions times spherical harmonics. In the interstitial region II, plane wave's expansion is used. Each plane wave is augmented by an atomic-like function inside the atomic sphere and matched at the atomic boundary. However, there is no shape restriction on the density and potential. The potential in LAPW method in the following form:

$$V(r) = \begin{cases} \sum_{lm} V_{lm}(r) Y_{lm}(\hat{r}) & \text{Inside sphere} \\ \sum_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} & \text{Outside sphere} \end{cases}$$

In this paper, we present the density of states (DOS) and the band structure for Nd atom at different sites, using spin-polarized method excluding the spin-orbit coupling.

2. METHOD OF CALCULATIONS

Nd₂Fe₁₄B crystal is a tetragonal unit cell with a space group P4₂/mnm, structure No. 136 [see Ref. 10, 11]. In one-unit cell, there are two kinds of 8Nd atoms, labeled as 4Nd(f) and 4Nd(g), respectively, six kinds of 56 Fe atoms, labeled as Fe (c), Fe (e), Fe (j1), Fe (j2), Fe (k1), Fe (k2), respectively, and only one kind of 4B atoms, labeled as B (g). We used the lattice constants and the fourteen atomic position parameters for Nd₂Fe₁₄B at 77K [see Ref. 12]. The experimental values used in our calculations are a= 8.802, c= 12.179 Å [5,6]. The Generalized Gradient

Approximation (GGA) of Perdew, Burke and Ernzerhof [13,14] used for correlations and exchange potentials as implemented in the Wien2k code [15]. Self-consistent calculations performed with 30 k-points in the irreducible Brillouin zone. We used the muffin tin (MT) sphere radii $R_{MT}^{Nd} = 2.5$ a.u., $R_{MT}^{Fe} = 2.09$ a.u., $R_{MT}^B = 1.85$ a.u and the cut-off energy parameters RKmax and Gmax of 7 and 14 respectively. 4f states in rare earths are highly localized and are very difficult to include the band-structure calculation. Fortunately, their photoemission spectra are reasonably well understood with a transition-state analysis [16,17] and renormalized atom approach [18]. Because of this and the fact that the non-4f parts of the experimental electronic structure are similar 4f states in Nd₂Fe₁₄B were included in the valence and core states. Both core and valence states are the frozen self-consistent atomic states. There are nine valence states per site consisting of s, p and d orbital. With 68 atoms per unit cell, this leads to 612×612 overlap and Hamiltonian matrices. The self-consistent spin-polarized potential parameters are based on the zero-wave-vector (K~0) electronic structure results. Because of the extremely large size of the unit cell so in our work, the 4Nd f electrons are considered as valence electrons and are treated as self-consistent. Furthermore, we used a small FPLAPW basis set for 8Nd atoms and small k-points for the Brillouin-zone integration.

3. RESULTS AND DISCUSSIONS

3.1 Density of States of Nd₂Fe₁₄B

We first performed spin polarized calculation using GGA but without including spin-orbit coupling. Figures (1,2) display the majority and minority density of states (DOS) for Nd atom at different sites in order to examine closely the f orbital. The highly localized peaks for Nd atom on f and g sites are located and clustered around EF. The 4f orbital in rare-earth is very important in deciding the properties of Nd₂Fe₁₄B. As shown in Figs.1 (a, b), We calculated the majority and minority DOS. The spin up in two Nd atoms on f site forms a narrow peak clustered around EF as shown in Fig. 1a. While the spin dn in Nd atom on f site, the peak found to be located above the EF as shown in Fig. 1b. Also as shown in Figs.2 (c, d), We calculated the majority and minority DOS. The spin up in two Nd atoms on g site forms a narrow peak clustered around EF as shown in Fig. 2c. While the spin dn in Nd atom on g site, the peak found to be located above the EF as shown in Fig. 2d. We note that peak for Nd atom on f site is longer than the peak for Nd atom on g site. We note that peak for Nd atom on f site is longer than the peak for Nd atom on g site. The Fe-site moments are in good agreement with two reported results of neutron scattering experiments, one with a single crystal [19] and on powder samples [20]. The average Fe moment is 2.38 μB per site compared to the experimental values ~ 2.57 μB per site [19]. The total magnetic moment calculated for Nd₂Fe₁₄B is ~ 46.62 μB per formula unit (FU). The total magnetic moment value is close to quoted experimental values of ~35.0 μB /FU or 37.1 μB /FU [19, 20].

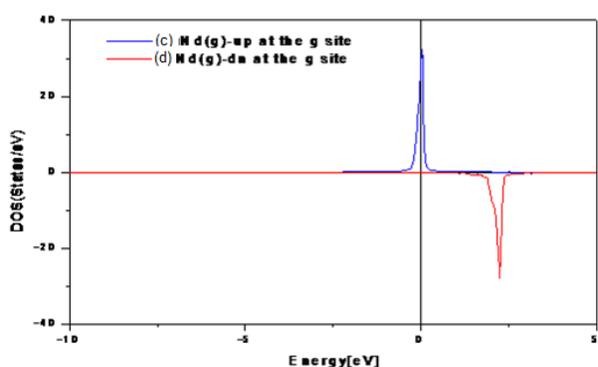


Figure 2: spin-up and spin-dn density of states (DOS) for Nd (g) atom at the g site versus the Energy : (a) Nd-up at g site; (b)Nd-dn at g site.

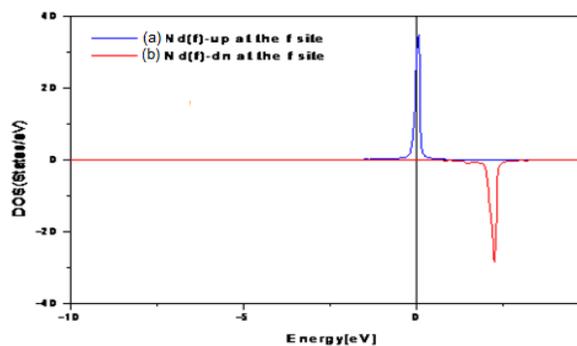


Figure 1: spin-up and spin-dn density of states (DOS) for Nd(f) atom at the f site versus the Energy : (a) Nd-up at g site;(b)Nd-dn at f site.

3.2 The Band Structure of Nd₂Fe₁₄B

Figures (3, 4) displays the band structures with just DFT-GGA for Nd atom. Each peak in DOS means that many wave vectors have the same eigen value. So that we note that the Nd atom on f site forms a narrow flat band at EF as

shown in Fig. 3. This flat band structure corresponds to a high density of states. On the other hand, in the Fig. 4, the peak in DOS located above E_F , means a high density of states as reflected in the band structure. Most of the DOS at E_F is contributed by the Nd sub-lattice.

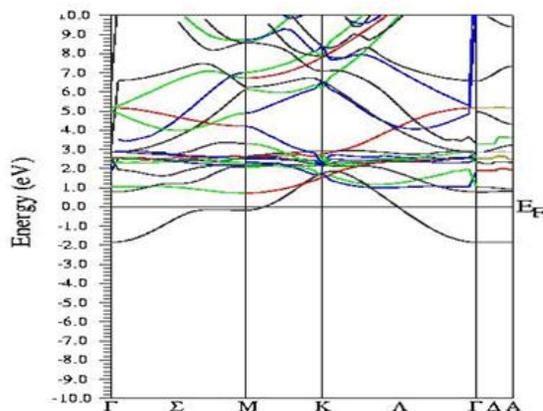


Figure 4: the band structure (Minority-spin band) for Nd atom at f site.

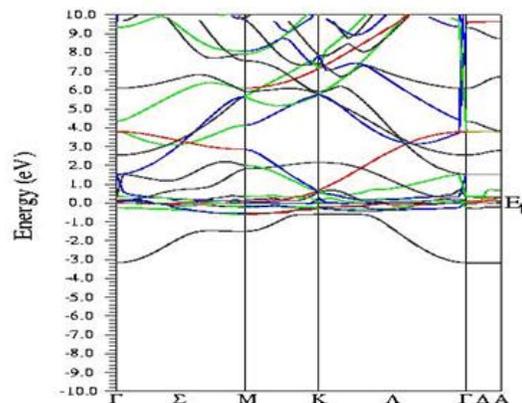


Figure 3: the band structure (Majority-spin band) for Nd atom at f site.

4. CONCLUSIONS

We performed a systematic ab initio calculation on Nd₂Fe₁₄B using spin polarized. The LDA + U scheme has been used and available in the Wien2k code. We calculated the majority and minority DOS for two Nd at 4f and 4g sites as shown in Figures in order to examine closely the f orbital in the two Nd at different sites. The total magnetic moment calculated for Nd₂Fe₁₄B is (46.62 μ B/FU) and the average Fe moment is (2.38 μ B); both numbers are close to the experimental values of 35.0 μ B/FU and 2.57 μ B respectively.

REFERENCES

- [1] K. S. V. L. Narashimhan, *J. Appl. Phys.* **57**, 4081 (1985).
- [2] J. Inoue and M. Shimizu, *J. Phys. F* **16**, 1051 (1986).
- [3] T. Itoh, K. Hikosaka, H. Takahashi, T. Ukai, and N. Mori, *J. Appl. Phys.* **61**, 3430 (1987).
- [4] B. Szpunar, W. E. Wallace, and J. Szpunar, *Phys. Rev. B* **36**, 3782 (1987).
- [5] Z. Q. Gu and W. Y. Ching, *Phys. Rev. B* **36**, 8530 (1987).
- [6] X. F. Zhong and W. Y. Ching, *J. Appl. Phys.* **67**, 4768 (1990).
- [7] D. J. Sellmyer, M. A. Engelhardt, S. S. Jaswal, and A. J. Arko, *Phys. Rev. Lett.* **60** 2077 (1988).
- [8] S. S. Jaswal, *Phys. Rev. B* **41**, 9697 (1990).
- [9] W. Kohn, and L. J. Sham, *Phys. Rev. A* **1133**, 140 (1965)
- [10] J. F. Herbst, J. J. Croat, F. E. Pinkerton, and W. B. Yelon, *Phys. Rev. B* **29**, 4176 (1984).
- [11] D.J. Singh, *Phys. Rev. B* **43**, 6388 (1991).
- [12] J. F. Herbst, J. J. Croat, and W. B. Yelon, *J. Appl. Phys.* **57**, 4086 (1985).
- [13] J. P. Perdew, Y. Wang, *Phys. Rev. B* **45**, 13244 (1992).
- [14] J. P. Perdew, K. Burke, M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [15] P. Blaha, K. Schwarz, G. K. H. Madsen, K. Kvasnicka, J. Luitz, Wien2k, Karlheinz Schwarz, Technische Universität wien, Austria “an Augmented Plane Wave + Local orbitals program for calculating crystal properties”, (2001).
- [16] M.R.Norman, D.D.Koelling, and A.J.Freeman, *Phys.Rev.B* **31**, 6251 (1985).
- [17] S.S.Jaswal, D.J.Sellmyer, M.Engelhardt, Z.Zhao, and A.J.Arko, *Phys.Rev.B* **35**, 996 (1987)
- [18] J.F.Herbst and J.W.Wilkins, in *Handbook on Physics and Chemistry of Rare Earths*, edited by K.A.Gschneider, L.Eyring, and S.Hufner (Elsevier, New York, 1987), Vol.10, p.321.
- [19] D. Givord and H. S. Li, *J. Appl. Phys.* **57**, 4100 (1985)
- [20] J. F. Herbst, J. J. Croat, and W. B. Yelon, *J. Appl. Phys.* **57**, 4086 (1985).