

AB INITIO CALCULATIONS OF MAGNETIC PROPERTIES OF THE INTERSTITIALLY DOPED YFe_{11}Mo COMPOUND

E. E. Kokorina^{*}, *M. V. Medvedev*, *I. A. Nekrasov*^{**}

*Institute of Electrophysics Russian Academy of Science
620016, Ekaterinburg, Russia*

Received July 19, 2015

The recent increase in the number of studies of $\text{RFe}_{11-x}\text{M}_x$ compounds is related to their promising application as permanent magnets. However, the insufficiently high value of the Curie temperature T_C of these compounds is a barrier to their widespread use. The increase in the Curie temperature of these compounds is achieved by doping with the light nonmetallic atoms such as hydrogen, nitrogen, and carbon. In this paper, it is shown numerically that this doping leads to drastic changes of the electronic band dispersions in a wide energy region around the Fermi level. This in turn changes values of the magnetic moments of ions and Heisenberg exchange interaction parameters. The values of ab initio calculated magnetic moments and direct exchange interaction parameters allow to calculate the Curie temperatures for both parent and nitrogen-doped compounds within the mean-field approach to the Heisenberg model in the sample of YFe_{11}Mo , a typical representative of the $\text{R}(\text{Fe},\text{M})_{12}\text{L}$ class. Theoretical values of T_C obtained for YFe_{11}Mo and $\text{YFe}_{11}\text{MoN}$ (514 K and 723 K respectively) are consistent with experimental ones (472 K and 664 K) with an accuracy of 10%. Also, the calculated increase in T_C upon nitrogenization (about 200 K) is in good agreement with the experimental data.

DOI: 10.7868/S004445101602019X

1. INTRODUCTION

The discovery of relatively inexpensive intermetallic compounds Nd-Fe-B with high saturation magnetization has raised interest in the development of R-Fe-M systems (R = rare earth and $\text{M} = \text{Al}, \text{Ti}, \text{V}, \text{Cr}, \text{Mo}, \text{W}, \text{Si}$ is a transition metal or metalloid) to use them as permanent magnets. Among these systems, $\text{R}(\text{Fe},\text{M})_{12}$ compounds have attracted particular attention due to a relatively high Curie temperature (T_C), noticeable saturation magnetization, and large uniaxial magnetocrystalline anisotropy at room temperature. It has been established that the structure stabilizing element M plays a key role in the formation of $\text{R}(\text{Fe},\text{M})_{12}$ structures that do not exist in the pure RFe_{12} form [1]. Investigations of $\text{R}(\text{Fe},\text{M})_{12}\text{L}$ systems ($\text{L} = \text{N}, \text{C}, \text{H}$ is the interstitial atom) were mainly carried out under the expectation to enhance their technologically useful hard magnetic properties [2–4]. Also, a significant increase in the Curie temperature observed upon light-element doping is an important feature for technological appli-

cations. To our knowledge, however, some phenomena related to these compounds are yet to be explained. In particular, the elementary lattice increases in volume upon doping, which in its turn decreases the electronic shell overlapping and corresponding exchange interactions. The latter may reduce the Curie temperature. But it was shown that, on the contrary, T_C increases with doping (see, e. g., Ref. [4]).

We note that a structure-stabilizing element M affects the magnetic properties of the compounds under investigation [5]. To reveal the role of the interstitial element L , it seems pertinent to study the system with a minimum amount of the third element M . In this paper, we investigate $\text{R}(\text{Fe},\text{M})_{12}\text{L}$ with $\text{M} = \text{Mo}$ and $\text{L} = \text{N}$. Among the series of RFe_{11}M compounds, the YFe_{11}Mo system has the most detailed experimental data on crystal structure [6], allowing us to investigate the exchange interactions for the compound both before and after the nitrogen absorption.

It is well known that the magnetic properties of ion-based intermetallic rare-earth compounds are improved with the absorption of some light ion ($\text{H}, \text{C}, \text{N}$). These improvements involve an increase in the Curie temperature and magnetization, and a more pronounced anisotropy [7]. Our next research will be focused on nitrogen-doped system. Among other light

^{*} E-mail: kokorina@iep.uran.ru

^{**} E-mail: nekrasov@iep.uran.ru

elements, the N absorption is known to provide the largest increase in T_C for the chosen RFe₁₁M systems [8]. The research challenge is to study the microscopic effect of doping on the exchange parameters, and consequently on the Curie temperature.

In the previous publications, we have elucidated a mechanism for increasing the Curie temperature by sp-metal doping [9] and the role of dumbbell ferrous ions in this process [10]. Hence, we illustrate that the origin of the increased Curie temperature due to interstitial doping in the YFe₁₁Mo compound is rather a complicated interplay of exchange interaction parameters due to the band structure modification. The whole picture cannot be simply mapped onto some toy model for such a complicated magnetic structure with many magnetic sites and sublattices.

The rest of the paper is organized as follows. In Sec. 2, we present a crystallographic structure of YFe₁₁Mo and YFe₁₁MoN together with some computational details. Section 3 is devoted to the results of ab initio calculations of magnetic properties performed for these compounds. Then the procedure of evaluation of the Curie temperature for both systems is described. In Sec. 4, we discuss the microscopic origin of the T_C increase with doping. A general conclusion is drawn in Sec. 5.

2. CRYSTAL STRUCTURE AND COMPUTATIONAL DETAILS

All R(Fe,M)₁₂ compounds crystallize in the same tetragonal structure of the ThMn₁₂ type [11] with the space group $I4/mmm$. YFe₁₁Mo has the lattice pa-

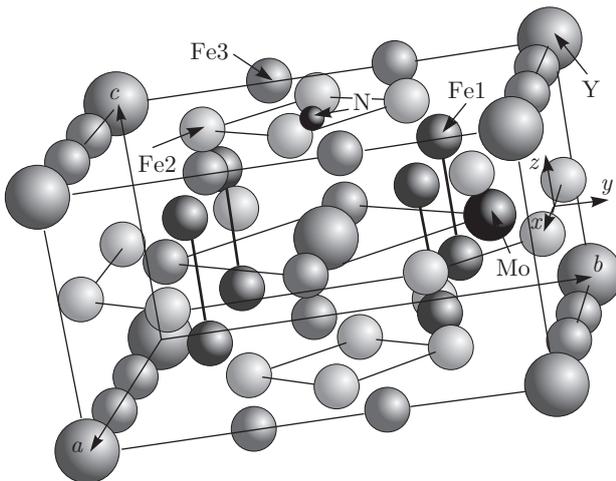


Fig. 1. Crystal structure of YFe₁₁MoN and N

rameters $a = b = 8.51 \text{ \AA}$ and $c = 4.77 \text{ \AA}$ [6]. In this structure, the rare-earth ion occupies the $2a$ (0, 0, 0) crystallographic sites. There are several crystallographically inequivalent positions of Fe ions: Fe1 ions almost fully occupy the $8f$ (0.25, 0.25, 0.25) and Fe2, the $8j$ (0.2769, 0.5, 0) sites, while the $8i$ (0.3587, 0, 0) sites are partially occupied by Fe3 and Mo ions (Fig. 1).

We note that nitrogenization of YFe₁₁Mo does not change its space group. Nitrogen occupies the interstitial position $2b$ (0, 0, 0.5). Due to the nitrogen absorption, the lattice parameters of YFe₁₁MoN increase compared to those of the parent compound YFe₁₁Mo, $a = b = 8.62 \text{ \AA}$ and $c = 4.79 \text{ \AA}$ [6]. Thus, interatomic distances responsible for the value of direct exchange interactions are also changed. In Fig. 2, we can see how distances between Fe ions nearest to nitrogen change upon doping. Most affected is the distance between Fe2–Fe2 ions, because they are the closest to the doping position.

The electronic structure of YFe₁₁Mo and YFe₁₁MoN was calculated by the LSDA+U method [12] using the TB-LMTO-ASA v.47 code (tight-binding, linear muffin-tin orbitals, atomic-sphere approximation) [13]. The Coulomb parameters derived with the constrained LDA method [14] are $U = 2.0 \text{ eV}$ and $J = 0.9 \text{ eV}$ for Fe [15], and $U = 2.8 \text{ eV}$ and $J = 0.5 \text{ eV}$ for Mo [16]. The calculations were performed in the Brillouin zone with $4 \times 4 \times 4$ spacing. Corresponding values of the Heisenberg exchange interaction parameters were obtained based on results of LSDA+U calculations with the method proposed in Ref. [18].

3. COMPARISON OF AB INITIO CALCULATED MAGNETIC PROPERTIES OF YFe₁₁Mo AND YFe₁₁MoN

A set of linear equations for T_C for the Heisenberg model of classical spin vectors in the mean-field approximation was obtained in Ref. [17]:

$$k_B T_C \sigma_a = \frac{S_a^2}{3} \sum_b \sum_{|\Delta_{ab}|} \tilde{J}_{ab}(|\Delta_{ab}|) z_{ab}(|\Delta_{ab}|) \sigma_b, \quad (1)$$

where Δ_{ab} is the distance between magnetic ions for $a, b = \text{Fe1, Fe2, Fe3, Mo}$; $\sigma_a = \langle S_a^z \rangle$ denotes the thermodynamic average of the z -projection of the classical spin vector \mathbf{S}_a corresponding to the magnetic moment $\mu_a = g\mu_B S_a$; $z_{ab}(|\Delta_{ab}|)$ is the number of Fe1, Fe2, Fe3, and Mo neighbors at the distance $|\Delta_{ab}|$ from the central ion; and \tilde{J}_{ab} is an exchange parameter between ions of types a and b . Ab initio calculated local and total magnetic moments of YFe₁₁Mo and YFe₁₁MoN

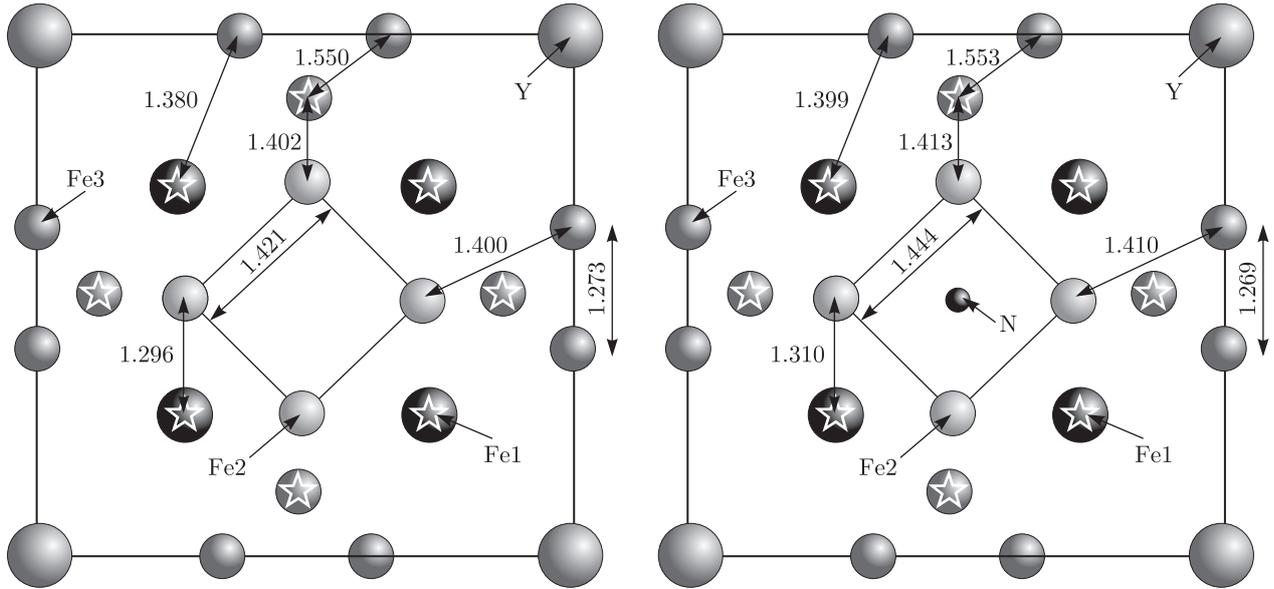


Fig. 2. Most physically important interatomic distances of YFe_{11}Mo (left) and $\text{YFe}_{11}\text{MoN}$ (right). Stars mark atoms of other layers. Distances are given in \AA

together with experimental data [6] are summarized in Table 1. In accordance with the experiment, the theoretical values of magnetic moments of ions of type Fe1 and Fe3 increase with doping, but those of Fe2, on the contrary, became weaker.

We first note that the energy of the exchange interaction between different sites of the magnetic lattice is presented in the Ref. [18] in the form $E_{ex}(\mathbf{l} - \mathbf{n}) = -2J_{ab}^L(\mathbf{l}_a - \mathbf{n}_b)\mathbf{e}_a(\mathbf{l}_a)\mathbf{e}_b(\mathbf{n}_b)$ as an exchange between two classical unit spin vectors $\mathbf{e}_a(\mathbf{l}_a) = (\sin \phi_a(\mathbf{l}_a) \sin \Theta_a(\mathbf{l}_a), \cos \phi_a(\mathbf{l}_a) \sin \Theta_a(\mathbf{l}_a), \cos \Theta_a(\mathbf{l}_a))$ and $\mathbf{e}_b(\mathbf{n}_b)$ regardless of the magnitude of the magnetic moments μ_a and μ_b at the sites \mathbf{l}_a and \mathbf{n}_b under consideration. Because the classical spin vector $\mathbf{S}_a(\mathbf{l}_a)$ is equal to $\mathbf{S}_a(\mathbf{l}_a) = S_a\mathbf{e}_a(\mathbf{l}_a)$, the relation between the exchange parameters J_{ab}^L calculated using the method in Ref. [18] and the exchange parameters \tilde{J}_{ab} of Eq. (1) is $2J_{ab}^L = \tilde{J}_{ab}S_aS_b$. Moreover, some authors [19] calculating exchange parameters for insulators prefer to write the exchange interaction energy as $E_{ex}(\mathbf{l} - \mathbf{n}) = -J_{ab}^M(\mathbf{l}_a - \mathbf{n}_b)\mathbf{S}_a(\mathbf{l}_a)\mathbf{S}_b(\mathbf{n}_b)$ in terms of the exchange parameters J_{ab}^M between classical spin vectors with the magnitude $S_a, S_b = 1/2$. It is easy to demonstrate that in using the method of Ref. [19] to calculate J_{ab}^M , our exchange parameters \tilde{J}_{ab} are related to J_{ab}^M as $\tilde{J}_{ab} = J_{ab}^M/(4S_aS_b)$.

The exchange integrals \tilde{J}_{ab} were calculated for all interaction pairs of Fe and Mo ions in the first coordination sphere. The first coordination sphere was chosen according to the following assumption: if we

consider a spherical layer with the radii in the range $r_1 = 1.262 \text{ \AA} < r < r_2 = 1.713 \text{ \AA}$ around a particular Fe1, Fe2, Fe3, or Mo ion, then all the nearest magnetic neighbors are within this coordination layer. Next comes an empty spherical layer without ions, $r_2 = 1.713 \text{ \AA} < r < r_3 = 2.009 \text{ \AA}$. The second spherical coordination layer is at $r > 2.190 \text{ \AA}$. Table 2 presents the exchange interaction parameters \tilde{J}_{ab} (in descending order of exchange values for YFe_{11}Mo) between the central ion Fe_a ($a = 1, 2, 3$) or Mo and another ion b from the first coordination layer. Here, $\tilde{J}_{23}(1)$ stands for the exchange parameter value between ions Fe2 and Fe3 at the nearest distance Δ_{23} between these ions (index 1 in the brackets), and $\tilde{J}_{23}(2)$ denotes the value of the exchange parameter between Fe2 and Fe3 ions at the second-order distance between them (index 2). Exchange integrals with Y ions are found to be negligibly small.

Evaluating the Curie temperature T_C using ab initio calculated data from Tables 1 and 2 and Eq. (1) gives for YFe_{11}Mo $T_C = 514.8 \text{ K}$, which is somewhat higher than the experimental value $T_C = 472 \text{ K}$ [7] (see also Table 2).

As we have mentioned, nitrogen takes the $2b$ position, which is surrounded by four Fe2 atoms in the $8j$ position. This nitrogen location leads to displacements of the neighboring Fe ions (see Fig. 2). To understand the consequences of that displacements for T_C , we evaluated the exchange interactions \tilde{J}_{ab} for both systems YFe_{11}Mo and $\text{YFe}_{11}\text{MoN}$.

Table 1. Ab initio calculated and experimental [6] local μ_a and total μ_{tot} magnetic moments (in μ_B) for YFe₁₁Mo and YFe₁₁MoN

Type of ion a	YFe ₁₁ Mo		YFe ₁₁ MoN	
	experiment	our calculations	experiment	our calculations
Y	0	0	0	0.15
Fe1	-2.15	-2.15	-2.38	-2.60
Fe2	-2.42	-2.28	-2.32	-2.30
Fe3	-2.36	-2.29	-2.43	-2.53
Mo	1.00	1.10	1.00	0.93
N	–	–	0	0
μ_{tot}	-24.36	-23.51	-25.09	-26.10

The most noticeable change in the distance is experienced by the pair Fe2–Fe2 (nearest to nitrogen doping position), in which exchange integrals naturally decrease as the distance increases. At the same time, another pair Fe3–Fe3(1) (and a pair with the same crystallographic position Fe3–Mo(1)) increased its exchange greatly with decreasing distance. But at the same time, pronounced changes occur within the exchange in pairs Fe2–Fe3(2) (and a pair with the same crystallographic position Fe2–Mo(2)) and in Fe1–Fe2, in which the exchange integrals increase significantly regardless of slightly growing distance. That may be explained by the effect of additional wave functions of nitrogen appearing in the vicinity of these pairs in the cell. We see that the interplay of changes in exchange parameters and distances is so complicated that the only possible way to make a conclusion is to estimate the influence on the Curie temperature by numerical analysis of system of equations (1). The exchange integrals obtained for YFe₁₁MoN lead to $T_C = 723.7$ K. This value is also somewhat higher than the experimental result $T_C = 664$ K [7]. Our calculations show a distinct increase in the Curie temperature with nitrogen doping, and the value of the increase (about 210 K) is practically the same as in experiment (about 190 K).

4. DISCUSSION

We try to understand the microscopic origin of the increase in T_C upon nitrogen doping. In the present calculations, the parameter of the effective direct exchange interaction J_{ij} between the nearest magnetic

sites i and j [12] is obtained as

$$J_{ij} = \sum_{\{m\}} I_{mm'}^i \chi_{mm'm''m'''}^{ij} I_{m''m'''}^j, \quad (2)$$

with the indices $\{m\} = m, m', m'', m'''$ being magnetic quantum numbers of the nl shells of i th and j th atoms. The spin-dependent potentials $I_{mm'}^i$ are expressed in terms of the single-particle potentials $V_{mm'}^\sigma$ ($\sigma = \uparrow$ or \downarrow) of the effective Hamiltonian of the LDA+U method [12]

$$I_{mm'}^i = V_{mm'}^{i\uparrow} - V_{mm'}^{i\downarrow}. \quad (3)$$

The effective inter-site susceptibilities $\chi_{mm'm''m'''}^{ij}$ are obtained in the second-order perturbation theory and are defined in terms of the LSDA+U eigenfunctions Ψ and eigenvalues $\epsilon_{nk\sigma}$ as

$$\begin{aligned} \chi_{mm'm''m'''}^{ij}(l) &= \\ &= \sum_{knn'} \frac{n_{nk\uparrow} - n'_{n'k\downarrow}}{\epsilon_{nk\uparrow} - \epsilon_{n'k\downarrow}} \Psi_{nk\uparrow}^{*ilm} \Psi_{nk\uparrow}^{jlm''} \Psi_{n'k\downarrow}^{ilm'} \Psi_{n'k\downarrow}^{*jlm''}, \quad (4) \end{aligned}$$

where the indices n and n' label the energy bands, and $n_{nk\sigma}$ is the occupancy of the $k\sigma$ state in the n th band, which is equal to 1 or 0.

In the initial compound YFe₁₁Mo, we calculate only the direct exchange interaction parameters J_{ij} in the nearest-magnetic-neighbor approximation. First, when a light atom N occupies an interstice in YFe₁₁Mo, the additional electrostatic potential arises in this interstice and the Fe and Mo atoms that surround this interstitial space are slightly displaced. This leads first to changes in the dispersion laws $\epsilon_{nk\sigma}$ in YFe₁₁MoN compared to those in the undoped compound YFe₁₁Mo. Second, essential changes in the eigenfunctions $\Psi_{nk\sigma}^{il}$ appear due

Table 2. LSDA+U calculated Heisenberg exchange interaction parameters \tilde{J}_{ab} for YFe₁₁Mo and YFe₁₁MoN, z_{ab} — number of atoms b around atom a , Δ_{ab} — corresponding distance. Last two lines show the theoretical and experimental [7] values of T_C

Exchange pairs	z_{ab}	YFe ₁₁ Mo		YFe ₁₁ MoN	
		$\Delta_{ab}, \text{\AA}$	\tilde{J}_{ab}, K	$\Delta_{ab}, \text{\AA}$	\tilde{J}_{ab}, K
Fe3–Fe3(1)	1	1.273	349.8	1.269	389.6
Fe3–Mo(1)	1		–699.2		–622.8
Fe2–Fe3(2)	2	1.402	160.2	1.413	204
			141.7		178
Fe2–Mo(2)	2		–201.4		–248
Fe2–Fe2	1	1.421	154.1	1.444	39.9
			69.7		19.7
Fe1–Fe2	1	1.296	150.7	1.310	207.9
			92.5		204.3
			44.2		166.1
			43.8		156.1
Fe2–Fe3(1)	1	1.400	149.1	1.410	98.6
			92.7		97.7
			73.4		87.4
Fe2–Mo(1)	1		–48.1		–95
Fe1–Fe1	2	1.262	141.2	1.267	102.8
Fe1–Fe3	1	1.380	134.4	1.399	125.7
			122.7		124.6
			85.0		80.7
Fe1–Mo	1		–212.8		–103
Fe3–Fe3(2)	2	1.550	101.5	1.553	80.2
Fe2–Mo(2)	2		32.8		35.4
T_C, K		514.8		723.7	
T_C^{exp}, K		472		664	

to doping because these must be expanded with respect to an extended set of atomic wave functions including the s and p wave functions of the interstitial N atom. As a result, in the doped compound YFe₁₁MoN, we calculated the direct exchange interaction parameters J_{ij} between the nearest magnetic ions anew, taking the modifications of the eigenvalues $\epsilon_{nk\sigma}$ and the eigenfunction $\Psi_{nk\sigma}^{ilm}$ with the light nonmagnetic interstitial atom into consideration. Then, using the obtained direct ex-

change interaction parameters, we evaluate the Curie temperature for YFe₁₁MoN.

Figure 3 (for YFe₁₁Mo) and Fig. 4 (for YFe₁₁MoN) show band dispersions and densities of states (DOS) calculated within the LSDA+U method. In the example of the band structures and DOS of YFe₁₁Mo and YFe₁₁MoN systems, we can see how deeply the electronic energy levels have been changed due to nitroge-

nization. We note that the calculated Curie temperatures for both compounds are somewhat higher than the measured ones. This is not surprising because it is common knowledge that the mean-field approximation gives overestimated values of the Curie temperatures for the three-dimensional Heisenberg ferromagnets with the nearest-neighbor exchange interactions compared with numerical methods or even with more sophisticated analytic methods of calculations, e. g., the random phase approximation. Nonetheless, the mean-field approximation represents rather well the Curie temperature change caused by changes of the exchange interaction parameters in compound YFe₁₁Mo due to doping.

Besides, an additional cause for the discrepancy between the theoretical evaluation of the Curie point T_C and the experimentally measured value T_C^{exp} can exist in the doped compound YFe₁₁MoN: it is produced in our calculations by disregarding additional indirect exchange interactions. It is evident that in the YFe₁₁MoN compound, the magnetic ions Fe and Mo adjacent to interstitial nitrogen atoms can be coupled not only with the direct exchange interactions but also with the indirect superexchange interactions through the agency of neighboring nonmagnetic N atoms (the indirect superexchange interaction that was proposed in Refs. [20] and [21]).

An additional complication for a microscopic analysis of systems under consideration is given by the well-known fact that the sign and the magnitude of the superexchange interaction parameter depend strongly on the superexchange angle Θ formed by p orbitals connecting a nonmagnetic atom to two neighboring magnetic ions [21, 22]. For instance, in iron-doped rare-earth orthochronites RCr_{0.99}Fe_{0.01}O₃, the effective superexchange Fe³⁺–O^{2–}–Cr³⁺ interaction parameter is positive (ferromagnetic) for $162^\circ < \Theta \leq 180^\circ$ and negative (antiferromagnetic) for $\Theta < 162^\circ$ [23]. In our case of the doped YFe₁₁MoN compound, the superexchange angles Θ are either right or acute for Fe–Fe pairs, and the interstitial superexchange interactions for these Fe atoms via N atoms are negative (antiferromagnetic) and rather small. We suppose that, as a

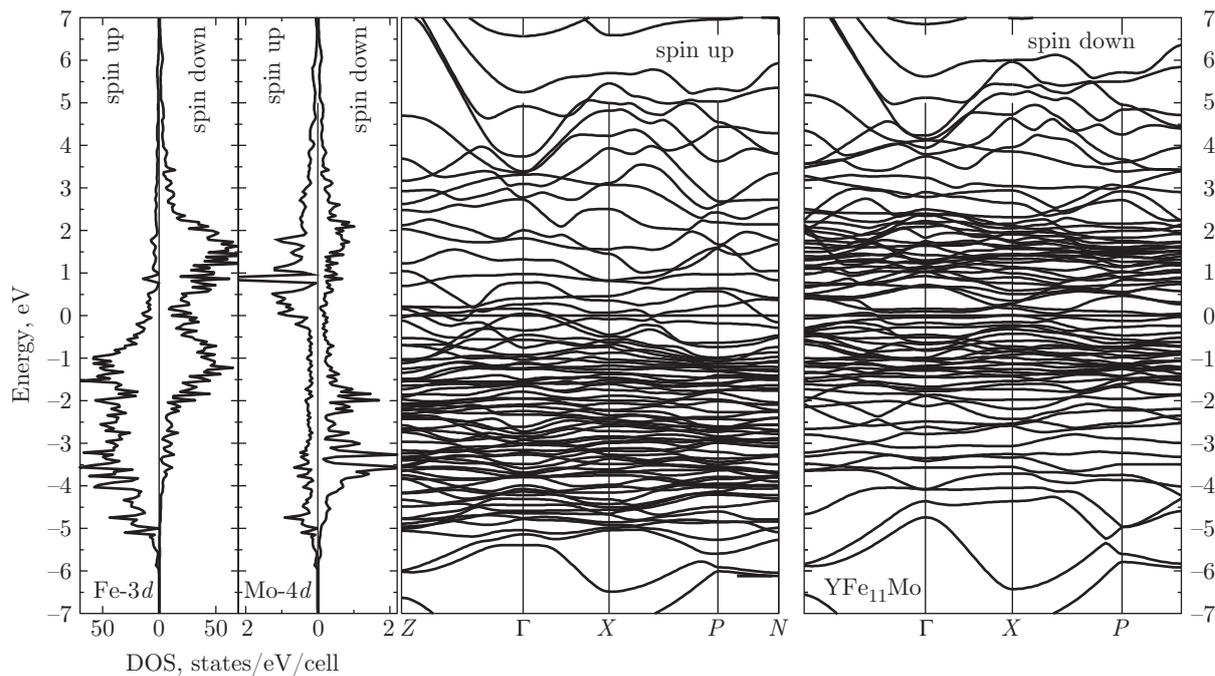


Fig. 3. LSDA+U calculated band dispersions (right) and densities of states (left) for $YFe_{11}Mo$. The Fermi level is at zero energy

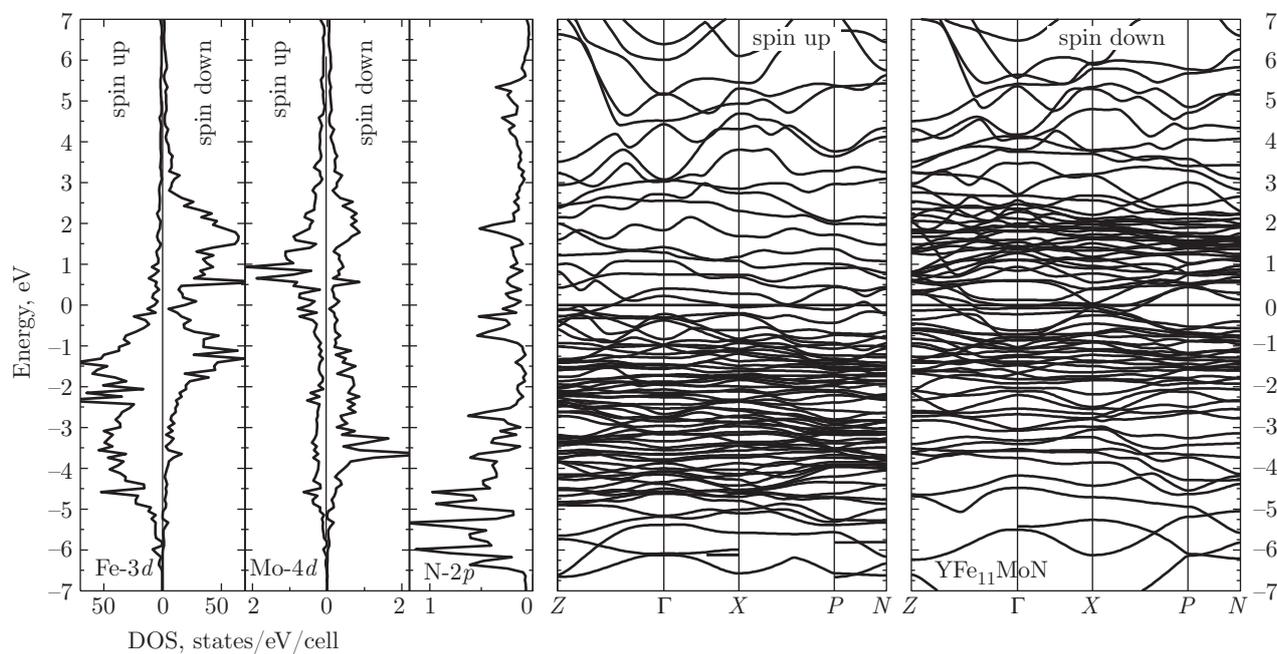


Fig. 4. LSDA+U calculated band dispersions (right) and densities of states (left) for $YFe_{11}MoN$. The Fermi level is at zero energy

result, each of the effective exchange parameters for these Fe–Fe pairs is the sum of large positive (ferromagnetic) parameter of the direct exchange interaction and a rather small negative parameter of the indirect superexchange interaction. This must slightly reduce some exchange parameters used in Eq. (1) and correspondingly the calculated value of the Curie temperature for the doped $\text{YFe}_{11}\text{MoN}$ compound.

However, we emphasize that the superexchange interactions appear only in the third-order perturbation theory terms [13, 24]. Therefore, the calculation of the superexchange interaction parameters is beyond the scope of the computational procedure [12] which is restricted to second-order perturbation theory terms and which is used in the present paper. It is evident that the calculation of superexchange interaction parameters needs a separate investigation.

5. CONCLUSION

The compound under consideration, YFe_{11}Mo (a typical representative of the $\text{R}(\text{Fe},\text{M})_{12}\text{L}$ class), reveals itself as a very complex structure, which is distinctly changed upon doping with light element N. It is unlikely that the microscopic description of changes in the magnetic properties may be reduced to any simple phenomenological model. An interplay of changed eigenvalues and eigenfunctions of Hamiltonian (1) arising due to the interstitial atom introduction and the corresponding crystal lattice relaxation leads to an increase in the direct exchange magnetic parameters upon doping. Because of a very complex magnetic structure, only numerical calculations may shed light on the electronic structure changes, which in its turn influence the exchange parameters and hence T_C .

Ab initio calculated values of magnetic moments and direct exchange interaction parameters (see Table 2) allow us to evaluate T_C for both YFe_{11}Mo and $\text{YFe}_{11}\text{MoN}$ compounds within the mean-field approach to the Heisenberg model. Theoretical values of T_C obtained for YFe_{11}Mo and $\text{YFe}_{11}\text{MoN}$ (514 K and 723 K respectively) are consistent with experimental ones (472 K and 664 K) with an accuracy of 10%. Also, the theoretical magnitude of the increase in T_C upon nitrogeization (about 200 K) is in good agreement with the experimental data.

This work was supported by the Russian Science Foundation (Project № 14-12-00502).

REFERENCES

1. Bo-Ping Hu, Kai-Ying Wang, Yi-Zhong Wang, Zhen-Xi Wang, Qi-Wei Yan, Pan-Lin Zhang, and Xiang-Dong Sun, *Phys. Rev. B* **51**, 2905 (1995).
2. N. Plugaru, J. Rubin, J. Bartolome, C. Piquer, and M. Artigas, *Phys. Rev. B* **65**, 134419 (2002).
3. I. S. Tereshina, G. A. Beskorovainaya, N. U. Pankratov, V. V. Zubenko, I. V. Telegina, V. N. Verbitskii, and A. A. Salamova, *Sol. St. Phys.* **45**, 101 (2003).
4. O. Isnard and V. Pop, *J. Alloys Comp.* **509S**, S549 (2011).
5. W. G. Chu, G. H. Rao, H. F. Yang, G. Y. Liu, and J. K. Liang, *Phys. Rev. B* **65**, 134424 (2002).
6. Hong Sun, Y. Morii, H. Fujii, M. Akayama, and S. Funahashi, *Phys. Rev. B* **48**, 13333 (1993).
7. Hong Sun, M. Akayama, and H. Fun, *Phys. Stat. Sol. (a)* **140**, K107 (1993).
8. S. A. Nikitin and I. S. Tereshina, *Sol. St. Phys.* **45**, 1850 (2003).
9. E. E. Kokorina, M. V. Medvedev, and I. A. Nekrasov, *Sol. St. Phenom.* **168–169**, 196 (2010).
10. M. V. Medvedev and I. A. Nekrasov, *Phys. Met. Metallogr.* **116**, 462 (2015).
11. K. H. J. Buschow, *Rep. Progr. Phys.* **54**, 1123 (1991).
12. V. I. Anisimov, F. Aryasentianawan, and A. I. Lichtenstein, *J. Phys. Condens. Matter* **9**, 767 (1997).
13. O. K. Andersen, *Phys. Rev. B* **12**, 3060 (1975).
14. O. Gunnarson, O. K. Andersen, O. Jepsen, and J. Zaanen, *Phys. Rev. B* **39**, 1708 (1989).
15. M. M. Steiner, R. C. Albers, and L. J. Sham, *Phys. Rev. B* **45**, 13272 (1991).
16. I. V. Solovyev, P. H. Dederichs, and V. S. Anisimov, *Phys. Rev. B* **50**, 16861 (1994).
17. A. V. Lukoyanov, E. E. Kokorina, M. V. Medvedev, and I. A. Nekrasov, *Phys. Rev. B* **80**, 104409 (2009).
18. A. I. Lichtenstein, M. I. Katsnelson, V. P. Antropov, and V. A. Gubanov, *J. Magn. Magn. Mater.* **67**, 65 (1987).
19. V. V. Mazurenko, F. Mila, and V. I. Anisimov, *Phys. Rev. B* **73**, 014418 (2006).
20. H. A. Kramers, *Physica* **1**, 182 (1934).
21. P. W. Anderson, *Phys. Rev.* **79**, 350 (1950).
22. J. B. Goodenough, *Phys. Rev.* **100**, 504 (1955).
23. A. S. Moskvina, N. S. Ovanesyan, and V. A. Trukhtanov, *Hyperfine Interactions* **1**, 265 (1975).
24. M. Shimizu, *Progr. Theor. Phys.* **8**, 416 (1952).