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Electronic structure and magnetic properties of $CoFe_3N$, $CrFe_3N$ and $TiFe_3N$

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Abstract

In this work, self-consistent band structure calculations were performed for the nitrides $CoFe_3N$, $CrFe_3N$ and $TiFe_3N$ at several lattice parameters to investigate the influence on the electronic and magnetic properties of Fe_4N due to the substitution of Fe atom by cobalt, chromium and titanium, as well as to study the behavior of the magnetism of these materials with pressure. In this study, we have employed the Linear Muffin-Tin Orbital (LMTO) method and our results show that $CoFe_3N$ is ferromagnetic with $2.26\mu_B$ and $2.07\mu_B$ as the magnetic moments at Co and Fe sites. On the other hand, $CrFe_3N$ is ferrimagnetic with a transition to a ferromagnetic order at high volume. Ferromagnetic calculations for $TiFe_3N$ give null magnetic moment, that is, the nonmagnetic state is the stable phase with a transition to a ferrimagnetic order at high volume as well. The magnetic hyperfine field (the Fermi contact) and the Isomer shift were also studied as a function of the lattice parameter for the $CoFe_3N$ and the $CrFe_3N$ nitrides. © 2001 Elsevier Science B.V. All rights reserved.

Keywords: Perovskite nitrides; Electronic structure; Magnetic properties; Hyperfine fields

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1. Introduction

In the last few years, several experimental and theoretical studies have been carried out on the electronic, magnetic, mechanical and crystallographic properties of iron-based nitrides [1–14]. These nitrides are very important due to their possible industrial applications: high nitrogen steels present good mechanical and corrosion resistance; transition metal nitrides may be used as hard metals to make wear-resistant materials (also due to the magnetic properties of these nitrides). Iron nitrides (γ'-Fe_4N and α''-$Fe_{16}N_2$), are characterized by their high saturation magnetization and low coercivity [1,2] and many papers are devoted to enhancing the magnetic qualities of the perovskite nitride, γ'-Fe_4N, as a coercive field by metallic substitutions [3–5]. In this sense, the effects of different substitutions on $M_xFe_{4-x}N$ ternary perovskite nitrides (where M=Fe, Mn, Au, Ag, Sn, Pd, Ni, Pt, In, Zn, Cu) have been reported where Mössbauer spectroscopy, magnetic, X-ray and neutron diffraction techniques were used [6–14]. The perovskite γ'-Fe_4N nitride is fully ordered with a simple crystallographic structure and it is a stable nitride, with iron atoms occupying the corner (FeI) and the face centered positions (FeII) and the nitrogen atoms, the body center positions. It is known that few atoms can substitute for iron atoms at the corner of the cube if their chemical affinity for nitrogen atoms is weaker than iron–nitrogen affinity. The chemical affinity between nitrogen and another metal atom increases if this atom is to the left side of iron in the periodic table. Furthermore, atoms on the right side of iron in the periodic table can be used to substitute iron in some iron nitrides in an ordered disposition, giving fully ordered compounds such as $PdFe_3N$, $AuFe_3N$, $PtFe_3N$ and $NiFe_3N$ since these atoms replace the iron at the corner position (zero nitrogen as nearest neighbors). In spite of several experimental difficulties to obtain other ordered substituted iron nitrides, many ternary iron nitrides ($Me_xFe_{4-x}N$) can be obtained by mechanical alloying [10,11,13,14] and theoretical studies have been reported on the electronic structure of fully ordered substituted iron nitrides by means of self-consistent band-structure calculations within the Local Spin Density approximation [8,11,13–21].

In this study, we made theoretical studies to get a clear understanding of the influences in the electronic and magnetic properties of Co, Cr and Ti substitutions in γ'-Fe_4N. Our interest in these metallic substitutions is

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based on the following reasons: ternary iron–cobalt nitride compounds were recently obtained by mechanical alloying [22]; titanium and chromium binary nitrides are well known with respect to their chemical, mechanical, electronic and magnetic properties (TiN is a compound with electrical conductivity of a good metallic conductor and the hardness of diamond). These binary nitrides (CoN, CrN and TiN) have been investigated recently by sophisticated synthesis and characterization techniques [23–28] and theoretical studies on electronic and magnetic properties also have been reported using first principles APW and the TB-LMTO-ASA methods [29,30]. However, little is known about iron-based ternary nitrides with cobalt, chromium and titanium substitution. In this sense, crystallographic and magnetic properties of (Fe,Ti)–N films were reported recently showing that the formation of the magnetic iron nitride phases is sensitive to the titanium doping concentration [31]. It was also shown that Ti doping can improve the thermal stability temperature of α''-$Fe_{16}N_2$ [32,33]. In the case of Co and Cr metals, thin films of CoFeN and CrFeN were prepared by the sputtering method and their structural and magnetic properties were investigated [34–36]. Thus, despite experimental difficulties to obtain ordered $CoFe_3N$, $CrFe_3N$ and $TiFe_3N$ from the theoretical point of view, these systems offer an interesting field of investigation on the electronic and magnetic properties of γ'-Fe_4N upon iron substitution by other transition metals.

Linear Muffin-Tin Orbital calculations [37,38], within the atomic spheres approximation (LMTO-ASA), were performed to study the magnetic and electronic structures of $CoFe_3N$, $CrFe_3N$ and $TiFe_3N$ ordered nitrides. For these calculations we took the crystal structures of these compounds as simple cubic, where the Co(Cr,Ti) atoms occupy the corner sites and the Fe atoms, the face-centered positions, while the nitrogen atoms occupy the body-centered sites. We performed spin-polarized LMTO calculations using the Vosko–Wilk–Nusair parameterization for the exchange-correlation energy of the electron gas [39]. Our LMTO calculations were made without spin-orbit interaction but included the combined correction terms [38]. For the fully ordered $CoFe_3N$, $CrFe_3N$ and $TiFe_3N$ nitrides the Wigner–Seitz Spheres (S_i) around Co (Cr) and Fe atoms were taken to be of equal size, and for Ti case we took $S_{Ti}=1.11S_{Fe}$. The Wigner–Seitz values were obtained using $4/3\pi\Sigma S_i^3=a^3$ (where a is the lattice parameter). For the nitrogen we take $S_N=0.5S_{metal}$ in the cobalt, chromium and titanium case. The overlap between Co(Cr) and Fe muffin-tin spheres is $0.066a$ and, between N and Fe spheres, it is $0.080a$. There is no overlap between Co(Cr) and N spheres. For the titanium case, the overlap between Ti and Fe muffin-tin spheres is $0.080a$ and, between N and Fe spheres, it is $0.082a$. There is no overlap between Ti and N muffin-tin spheres. The one-electron potentials were self-consistently obtained using reciprocal space sums with 455 **k**-points. The self-consistent cycles were carried out until energy convergence on a scale better than 0.5 mRy was achieved. The solutions of the Schrödinger equations use s, p, d and f LMTO basis functions for metals (Fe, Ti) and s, p and d basis functions for Cr and nitrogen atoms. The densities of states (DOS) were calculated as a sum of delta functions for a fixed number of mesh points and the energy window was divided into a mesh of 1500 points.

2. Results and discussion

Total energy calculations were made for several lattice parameters to obtain the equilibrium volume. The calculated binding curves for the ordered nitrides are shown in Fig. 1 (relative total energies in Ry and lattice parameters in atomic units). The binding curves for $CoFe_3N$ and $CrFe_3N$ were obtained through an analytical fitting of the calculated total energies to a fourth degree polynomial and for $TiFe_3N$ to a third degree polynomial. The corresponding equilibrium lattice constants, bulk moduli, Fermi energies, magnetic moments and the hyperfine parameters are shown in Table 1. Clearly, as expected, there is a lattice contraction relative to the γ'-Fe_4N (experimental lattice constant $a=7.1713$ a.u.), due to the substitution of Fe atoms (at corner positions) by Ti and Cr atoms and, an expansion of the lattice parameter in the case of cobalt

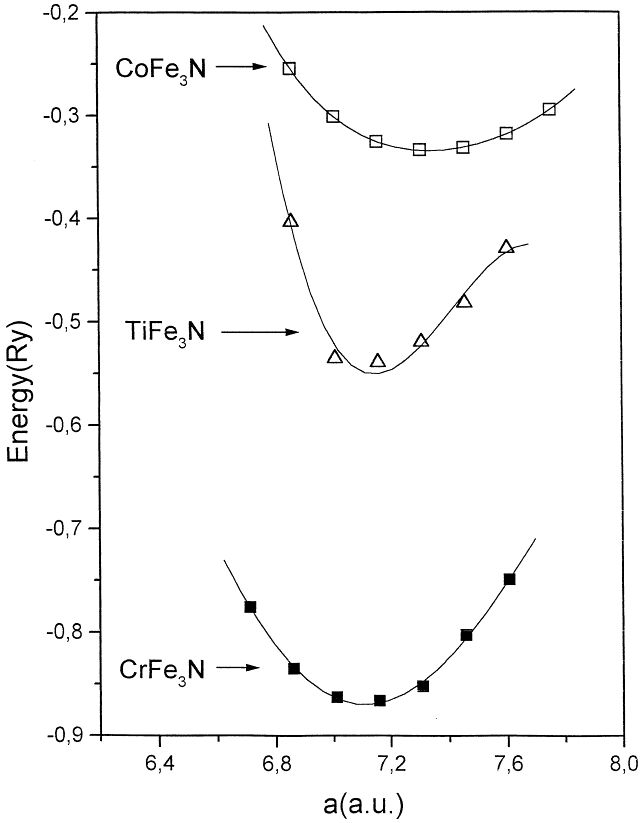

Fig. 1. Total energy curves (Ry) versus lattice parameter (atomic units) for the Co (Cr, Ti)Fe_3N nitrides (relative energies).

Table 1
Theoretical parameters for $CoFe_3N$, $CrFe_3N$ and the $TiFe_3N$ nitrides[a]

	a	μ_{Fe}	μ_{metal}	E_F	B	H_{FC}	IS
$CoFe_3N$	7.3430	2.07	2.26	0.696	111	−23.1	0.562
$CrFe_3N$	7.1094	−0.59	2.56	0.818	267	16.5	0.307
$TiFe_3N$	7.1450	0.00	0.00	0.825	596	0.00	0.333

[a] Parameters are: equilibrium lattice spacing a (atomic units); magnetic moments μ (Bohr magnetons) at iron and metal sites (Co, Cr); Fermi energy E_F (Ry); bulk modulus B (GPa); Fermi contact H_{FC} (Tesla) and Isomer Shift IS (mm/s) at iron sites.

substitution. On the other hand, a comparison with a previous [21] LMTO-ASA calculation which gives 7.0860 a.u. as the theoretical equilibrium lattice parameter for Fe_4N, shows an expansion of the lattice constant for Ti, Cr and Co substitution. Furthermore, the calculated bulk modulus for Fe_4N is 406 GPa [21] (the experimental value is 198 GPa [40]) and from Table 1, it is clear that only Ti substitution gives a bulk modulus which is greater than that of Fe_4N. At this point we stress that the total energy function, which is minimized in standard LMTO-ASA calculations, is a function of the atomic spheres approximation for the charge density for fixed atomic-sphere radii. The deviation from proper total energy is minimal when the spheres can be closely packed as in f.c.c. or h.c.p. arrangements (which is not the case for the nitrides under study) and even in these cases the choice of the sphere radii can be critical. This could explain the high values for the bulk modulus obtained with LMTO-ASA calculations.

Table 1 shows that $CoFe_3N$ is ferromagnetic and the magnetic moments at cobalt sites are greater than that in pure metal cobalt. At Fe sites, the magnetic moments shows a small deviation from the value at the face centered position of Fe_4N which is $2.10\mu_B$ [8,15,20]. Hence, for cobalt substitution we obtain $8.45\mu_B$ as the magnetic moment per formula unit. For Fe_4N, the theoretical result is $9.40\mu_B$. Therefore, cobalt substitution gives a high magnetic moment per formula unit relative to the other metallic substitutions, e.g. $6.14\mu_B$ and $6.42\mu_B$ for $AgFe_3N$ and $AuFe_3N$ [11]; $7.44\mu_B$ for $PdFe_3N$ [16,19]; $6.00\mu_B$ for $SnFe_3N$ [18]; $7.20\mu_B$ for $NiFe_3N$ [16]; $7.76\mu_B$ for $PtFe_3N$ [41] and $3.60\mu_B$ for $ZnFe_3N$ [13]. Besides the structural differences, this high magnetic moment may be related to the recent experimental results of Wang et al. [34], where they reported a very high saturation magnetization of FeCoN films. Furthermore, Mössbauer spectra of $Co_xFe_{8-x}N$ $(0.4 \leq x \leq 2)$, which has a hexagonal structure [22], show that the hyperfine magnetic field increases with cobalt concentration, but, besides that, no magnetic measurements were done for these compounds. From the linear relation between the hyperfine field and the magnetic moments, certainly the magnetic moments must increase with cobalt content.

Contrary to the ferromagnetic order in the cobalt case, chromium substitution drastically changes the ferromagnetic order of Fe_4N. For $CrFe_3N$, the calculated magnetic moments at Cr and Fe sites are opposite in sign (Table 1) with a high magnetic moment at the Cr sites and a low magnetic moment at the Fe sites. That is, for $CrFe_3N$ we found a ferrimagnetic order, as in the case of Mn_4N [15] and other Mn-based nitrides [41]. To our knowledge, for iron substituted nitrides this magnetic behavior is present only in $MnFe_3N$ [19] with the magnetic moments at Mn and Fe sites equal to $-2.93\mu_B$ and $1.18\mu_B$, respectively. On the other hand, Table 1 shows that titanium substitution breaks down the ferromagnetism of Fe_4N with zero magnetic moments at the various sites and this system has a non-magnetic ground state, which was also observed for indium substitution [13]. Clearly these results show the connection between the magnetism and the geometrical arrangement of the atoms on a local scale. We notice that for the Co and Cr iron-based nitrides under study, the magnetic moments found at nitrogen sites were very small, being less than $0.05\mu_B$.

We have calculated the l-projected densities of states (l-DOS) at the theoretical equilibrium volumes to investigate the trends of the chemical bonds, from an itinerant model point of view, in the iron-substituted $CoFe_3N$, $CrFe_3N$ and $TiFe_3N$ nitrides. In Figs. 2–4 are shown the calculated d densities of states for both spin directions at Co, Cr, and Ti sites (solid lines) and at Fe sites (dash–dot

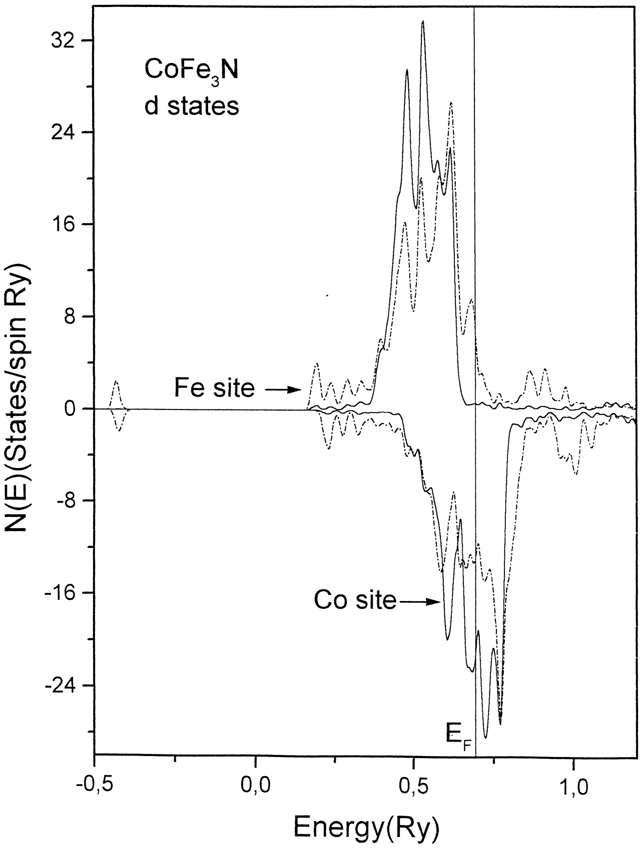

Fig. 2. The d-projected densities of states for spin-up and spin-down electrons at Fe sites (dash–dot line) and at Co sites (solid line) of the $CoFe_3N$. E_F is the Fermi energy.

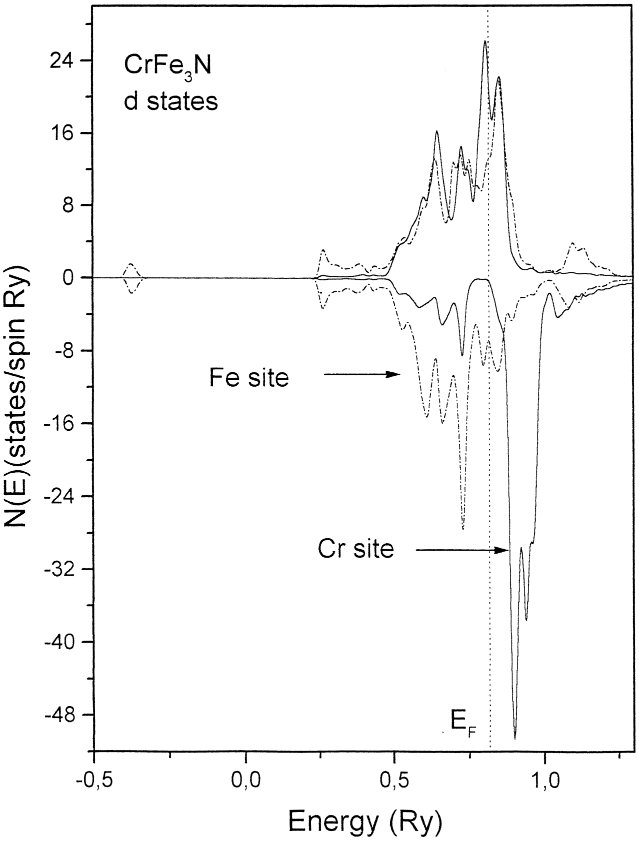

Fig. 3. The *d*-projected densities of states for spin-up and spin-down electrons at Fe sites (dash–dot line) and at Cr sites (solid line) of the CrFe$_3$N.

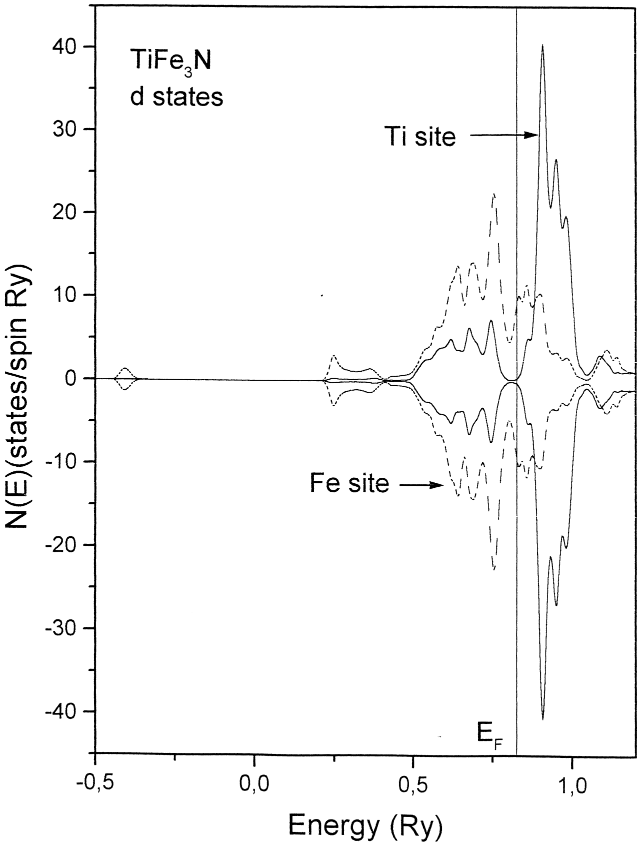

Fig. 4. The *d*-projected densities of states for spin-up and spin-down electrons at Fe sites (dash–dot line) and at Ti sites (solid line) of the TiFe$_3$N.

lines) for these nitrides. At Fe sites (for the three nitrides), the appearance of bonding states at low energies (near −0.5 Ry) reflects the interaction between nitrogen s states and iron d states since the *s*-DOS at N sites (not shown) has significant values in the energy range −0.5 to −0.30 Ry indicating the localized character of the s states at these sites. Our results for *s* and *p*-DOS indicate also a strong interaction between iron s and p states with nitrogen s and p states. These N–Fe and also the small Co(Cr,Ti)–Fe interactions broaden the *l*-DOS at Fe sites and charge transfer from N and Co(Cr,Ti) to Fe atoms populate the states at Fe sites. Contrary to the evident strong N–Fe interaction, the *l*-DOS at Co(Cr,Ti) sites, indicate that the (Co,Cr,Ti)–N interactions are very weak and more subtle, in the sense that we observe the appearance of pCo(Cr,Ti) bonding states in a narrow energy range, within the energy range where the *p*-DOS (not shown) of N sites is prominent. These general features of *l*-DOS at various sites were also reported earlier [11,13,16,19] and indicate the metallic character (itinerant electrons) of these and other iron-substituted nitrides, that is, the use of ionic and covalent models are not appropriate to give a good description of their electronic structures. The formation of magnetic moments out of completely delocalized electrons is also explained with the aid of the *d*-DOS. From Fig. 2, it is easy to see that for the CoFe$_3$N, at Co and Fe sites the spin-up d states are fully occupied, and that some of the spin-down d states are empty. Therefore, we have a common d-band for spin-up electrons, but spin-down electrons are partially excluded from iron sites, which gives the calculated magnetic moment for each site (Table 1).

From Fig. 3 we see a different behavior of *d*-DOS for the CrFe$_3$N, which explains the ferrimagnetic order of this nitride. The spin-down d states at Cr sites are mostly empty while spin-up states are occupied giving the appreciable magnetic moment shown in Table 1. At the iron sites, there is an inversion with the spin-down d states slightly more occupied than that of spin-up states, which gives the small opposite magnetic moment at these sites. For the TiFe$_3$N the *d*-DOS shows clearly that both spin directions have equal occupation numbers and this system is non-magnetic.

To investigate the sensitivity of the magnetic moments against lattice spacing for the (Co,Cr,Ti)Fe$_3$N nitrides, we have calculated the magnetic moments for several lattice parameters, simulating pressure effects. Fig. 5 shows the behavior of the magnetic moments at Co, Cr, Ti and Fe sites as a function of the lattice spacing. For the CoFe$_3$N nitride the magnetic moment at Co sites remains almost

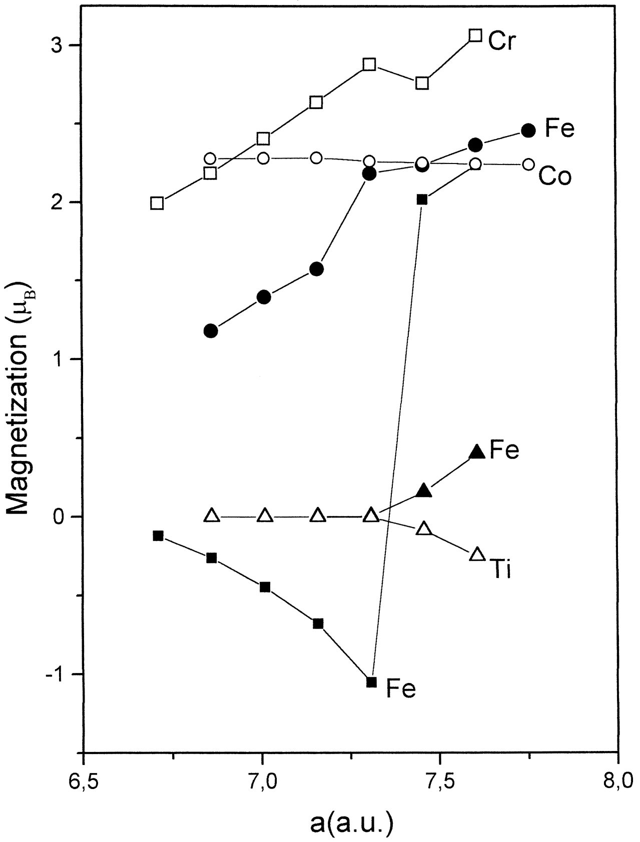

Fig. 5. The magnetic moments (in Bohr magnetons) as a function of lattice parameter at Fe (■) and Cr (□) sites for CrFe$_3$N; at Fe (●) and Co (○) sites for CoFe$_3$N and at Fe (▲) and Ti (△) sites for TiFe$_3$N nitride.

constant while at the iron sublattice there is a decrease of the magnetic moment. For γ'-Fe$_4$N, there is a collapse of the magnetic moment with pressure. That is, this system shows a transition from ferromagnetic state to a nonmagnetic state at low volume [18,20], which was also observed in other substituted iron nitrides [11,14,16,18,19] and is in good agreement with the experimental results on thermal expansion and forced magnetostriction [40,42], and applied pressure Mössbauer spectroscopy [43,44]. Hence, contrary to the other metallic substitutions (Pd, Ni, Sn, Au, Ag, Cu), the substitution of the iron atoms at corner positions by cobalt atoms preserves the magnetic moment of iron atoms at the face-centered positions with applied pressure. In the case of chromium substitution, a completely different magnetic behavior is observed as can be seen in Fig. 5. The magnetic moment at Cr sites decreases remaining finite at low volume, but at Fe sites the magnetic moment goes to zero. Therefore, for high pressure there is a magnetic transition from ferrimagnetic to ferromagnetic order, with magnetic moments defined only at the Cr sublattice. On the other hand, for high volumes (around $a=7.30$ a.u.) we observe an abrupt change in the magnetic moment at Fe sites which is now aligned with the Cr magnetic moment. Thus, the CrFe$_3$N nitride is ferromagnetic at high volume with a great magnetic moment per formula unit ($\cong 9.0\mu_B$). Our calculations with titanium substitution show a quite different behavior for the magnetism (Fig. 5). TiFe$_3$N is nonmagnetic at equilibrium and low volume, but for larger lattice constants there is a transition to a ferrimagnetic state. To our knowledge, this is the first time that such a transition has been observed in ordered substituted iron nitrides (ferrimagnetic→nonmagnetic). Ferrimagnetism was also found for manganese substitution [19], but MnFe$_3$N remains ferrimagnetic at larger volume and has a transition (at low volume) to a ferromagnetic state with zero magnetic moment at the iron sublattice as in the chromium case.

For CoFe$_3$N at equilibrium volume, the calculated magnetic hyperfine field H_{FC} (the Fermi contact contribution) at Fe sites was -23.0 Tesla. For the Cr case, H_{FC} has the opposite sign, $+16.5$ T (Table 1). The Isomer Shift (IS) was calculated using standard values [45] for the density of the s-electrons at the nucleus of the source. We obtained IS as 0.562 mm/s at Fe sites for cobalt and 0.307 mm/s for chromium substitution. In a previous calculation on γ'-Fe$_4$N [8], $H_{FC}=-24.4$ T and IS=0.390 mm/s were obtained at the face-centered iron atoms. Thus Co substitution lowers the Fermi contact (absolute value) but the IS value is increased. For the Co case, the increase in IS (at Fe sites) reflects the sensitivity of the s-electron density at Fe nuclei with the local arrangement of atoms. Due to d–d interactions between metals, there is an increase in the minority spin d-electrons and, since the density of s-electrons remain almost constant, the large value for IS (for CoFe$_3$N) comes from increasing the d-electron number.

Our theoretical results also indicate a strong dependence of H_{FC} and IS on the lattice spacing for CoFe$_3$N and CrFe$_3$N, as shown in Fig. 6. The observed decrease in H_{FC} may be related to the reduction of the contribution of the localized s-electrons to the spin density at iron nuclei. This behavior of H_{FC} and IS at Fe sites by shrinking the lattice spacing is very similar to that of gold and silver substitution [11] in Fe$_4$N. In fact, from Fig. 6 we see that the reduction of the IS value when Co atoms are substituted by Cr atoms can be viewed as a simulation of an applied pressure in CoFe$_3$N since an increase in s-electrons is equivalent to a reduction of d-electrons on the IS value. This increase in the density of the s-electrons at the nuclei at low volume was also observed by Paduani et al. [46] in their work on γ'-Fe$_4$N.

3. Conclusions

The electronic and magnetic structure of the fully ordered compounds CoFe$_3$N, CrFe$_3$N and TiFe$_3$N were studied using the LMTO method. Total energy calculations give the equilibrium lattice parameters for these nitrides.

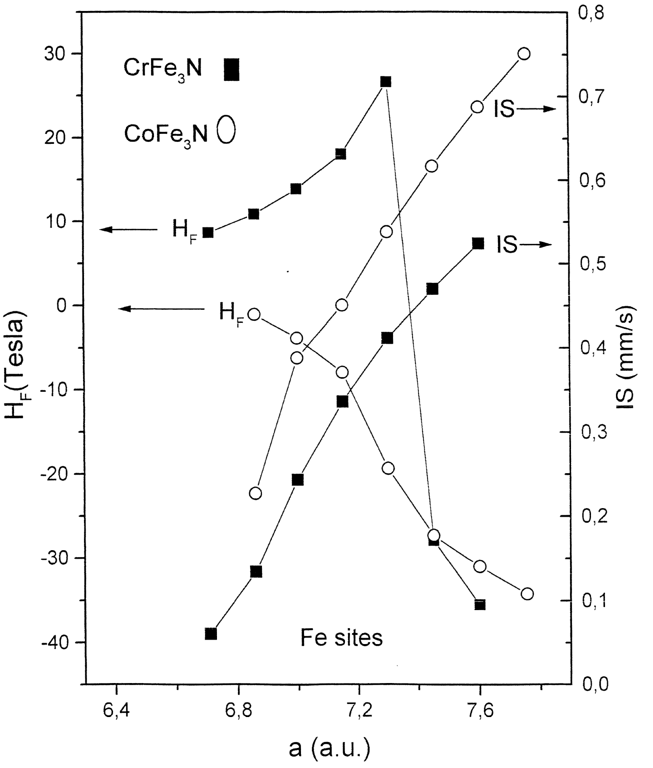

Fig. 6. The Isomer Shift and the Fermi contact at iron sites as a function of lattice parameter for $CoFe_3N$ and $CrFe_3N$ nitrides.

For $CoFe_3N$, the ground state is ferromagnetic and a comparison with Fe_4N nitride shows that the magnetic moment at Fe atoms at face-centered sites remains the same upon substitution of iron at corner positions by cobalt atoms. Cobalt substitution gives the higher magnetic moment per formula unit among other substituted iron nitrides and that is close to the value of the Fe_4N. In the case of $CrFe_3N$, we found a ferrimagnetic order with a small magnetic moment per formula unit. On the other hand, for $TiFe_3N$ at the theoretical equilibrium lattice constant, the system is nonmagnetic with no net magnetic moment at both Ti and Fe sites.

The behavior of the magnetic moments as a function of volume for these nitrides (or equivalently with pressure) showed that for low volume, ferromagnetism remains practically unaltered with cobalt substitution, contrary to the case of Fe_4N and other metallic substitution (as Pd, Sn, Au, Ag, Cu) where drastic variations of the magnetic moment were observed including a transition from ferromagnetic to a nonmagnetic state. For $CrFe_3N$, the magnetism is strongly dependent on the lattice spacing. At high volume this system is ferromagnetic with a great magnetic moment per formula unit. For the lattice spacing around 7.30 a.u. this nitride makes a remarkable transition to ferrimagnetic order due to an abrupt change in the magnetic moment at Fe sites, since there is only a smooth decrease of the magnetic moment at Cr sites. For lattice parameters below the equilibrium volume, the magnetic moment at Fe sites decreases in absolute value to zero, and since the magnetic moment at Cr sites remains finite, the system makes another magnetic transition from ferrimagnetic to ferromagnetic order but now with a low magnetic moment per formula unit. The ferromagnetism of Fe_4N nitride disappears with Ti substitution, that is, $TiFe_3N$ is nonmagnetic at equilibrium volume, but shows a transition to ferrimagnetic order at high volume with a small, opposite magnetic moment at Ti and Fe sites. The theoretical results at equilibrium volume for H_F and IS at Fe sites showed that Co lowers the Fermi contact relative to Fe_4N and increases the IS value. For Cr, H_{FC} has an opposite sign and a smaller IS value than that of Fe_4N. The hyperfine parameters for $CoFe_3N$ and $CrFe_3N$ also showed a strong dependence on the lattice parameter with a reduction of IS at low volume. This increase of s-electrons at the nuclei for high pressure is very similar to what occurs in Fe_4N, $AuFe_3N$ and the $AgFe_3N$ nitrides, and is in accordance with experimental results [11].

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