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Міжвузлові домішки Cr в залізі: мультифероїчні властивості

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INTERSTITIAL Cr IMPURITIES IN IRON: MULTIFERROIC PROPERTIES

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Міжвузлові домішки Cr в залізі: мультифероїчні властивості

З.А.Дурягіна, Н.Павленко, Н.Щербовськиx

Анотація. Виконано повну атомну релаксацію об'ємного фериту з 12,5%-ю концентрацією одноатомних міжвузлових домішок Cr періодично розташованих на ребрах комірок кубічної гратки Fe_α. Показано що структурна релаксація призводить до значних атомних зміщень і до формування паралельних ланцюжків почергово прокручених октаедрів Fe_6. Такі атомні зміщення ведуть до появи нового металічного стану який може бути визначений як мультифероїчний та напів-металічний. Як наслідок фрустрації магнітних моментів заліза домішками Cr, виникаючий просторово- неоднорідний розподіл магнітних моментів супроводжується появою статичної електричної поляризації. Властивості змодельованих в роботі сплавів міжвузлового типу можуть мати ряд важливих застосувань в спінтроніці та в багатофункціональних пристроях.

Interstitial Cr impurities in iron: multiferroic properties

Z.A.Duriagina, N.Pavlenko and N.Shcherbovskikh

Abstract. We perform a full atomic relaxation of the bulk ferrite with 12.5%-concentration of monoatomic interstitial Cr which is periodically located on the edges of cubic cell of Fe_α. We show that structural relaxation leads to significant atomic displacements and results in the formation of parallel chains of alternatively tilted Fe_6-octahedra. The atomic distortions result in the formation of a new metallic state which can be characterized as multiferroic with the electronic properties close to half-metallic. The static electric polarization appears due to inhomogeneous spatial distribution of magnetic moments caused by their frustration by Cr impurities. The properties of generated interstitial alloys can have important consequences for the applications in spintronic and multifunctional devices.

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1. Introduction

Last years demonstrated an increased activity in search for new materials with coexistent magnetism and ferroelectricity which are called multiferroics [1–3]. Due to emerging possibility to control the electric polarization by magnetic fields and, visa versa, spins by applied voltages, multiferroics open new perspectivesfor applications in multifunctional devices.

The mechanism of multiferroic phenomena is related to the magnetic origin of ferroelectricity induced by frustrated magnetic order. Due to inhomogeneous magnetic patterns, any weak relativistic or nonrelativistic spin-orbit magnetoelectric coupling can produce significant electric polarization. The prominent examples of such mangetoelectric coupling are rare-earth manganites $RMnO_3$ and RMn_2O_5 (R is a rare-earth ion or Y) [2, 4–6].

In search for new efficient multiferroic materials for technological applications in a wide series of long-term devices, the properties like hardness, corrosion, heat resistance and other types of mechanical and chemical durability are of central interest [7, 8]. It is worth noting that as it frequently appears in science and technology, some well known materials, when analyzed from different points of view and in combination with other compounds give rise to unexpected features not revealed previously.

As an example of such a new bahavior, we discuss in the present work an alloy Fe-Cr. Substitutional alloys Fe with Cr attracted strong attention of theory and experiment due to their magnetic properties, and especially due to local antiferromagnetism in the proximity of Cr [9–12]. In our work, we consider different type of alloys, namely, interstitial Fe-Cr alloys where the Cr impurities are located in the interstitial positions of the initially bcc lattice of Fe_α. The alloys Fe-Cr, doped by C, Ni and a wide variety of other compounds, are widely used as basic components for ferrite, martensitic and austenitic steels and responsible for their mechanical and physical properties. In the theoretical studies of intersitials in Fe-Cr, the different configurations of the interstitial configurations were calculated. Among them, a pair configuration $\langle 111 \rangle$ dumbbell is considered as the most energetically favourable which requires about 4.2 eV for its formation under irradiation [13]. In this work, we analyze monoatomic interstitial configurations with single Cr atoms on the edges of the bcc ferrite. As appears from the calculations of optimized structures, the energy gain for such configurations can approach 4.05 eV which makes this type of intersitial defects especially stable and robust.

It should be also noted that the fundamental difference between the industrial alloys and the alloys studied in the present work is the ordered character of the latters. In steels, due to their amorphic character, the impurities are distributed randomly. Moreover, the process of the hardening of steels proceeds through the surface treatment and is accompanied by formation of granular microstructure with the changed concentration of impurities and modified properties [14]. In contrast to this, in our generated systems the Cr impurities are located periodically in the cubic lattice of Fe_α. Due to substantial local forces, the atomic positions have to be structurally relaxed which produces patterns with unexpected microstructures and new properties. Last x-ray studies give a direct support of the presence of Cr in the interstitial positions of stainless steels which motivates the studies of interstitial Fe-Cr alloys.

In the present work we obtain that the optimized lattice microstructure has a clasterized or chain-like character where the chains of tilted Fe_6-octahedra are paralelly arranged along the x-axis. We show that the spatially inhomogeneous magnetic moments induce a nonzero electric polarization and lead to a coexistence of the magnetism and ferroelectricity. On the other hand, we find that the behavior of the relaxed system is close to half-metallic, with the density of electron states for one spin direction strongly suppressed near the Fermi level. This makes the generated systems perspective candidates for spin polarizers in spintronic applications. Furthermore, in the chain-like structures the relaxation leads to formation of spatial voids which can be used as channels for the diffusion of particles like N, Li, C and others. In our studies, we calculated diffusion barriers for N and discussed possible diffusion paths of nitrogen in these channels. In all the results, the structural relaxation plays a central role and must be inevitably considered in any realistic studies of such types of interstitial systems.

2. Structural relaxation of interstitial alloy Fe_α-Cr

To study Cr atoms in the interstitial positions of Fe_α, we generated a supercell which is based on a doubled 2×2 cubic cell of ferrite with Cr located on one of the edges of elementary cubic unit cell (see Fig. 1). In this way, the modelled structure Fe_8Cr corresponds to an interstitial Fe-Cr alloy with Cr concentration $n = 0.125$ which is typical for stainless steels. The presence of interstitial Cr leads to significant local forces acting on the neighbouring Fe atoms. To minimize the forces, the coordinates of all atoms have been relaxed which is achieved through the minimization of the total energy.

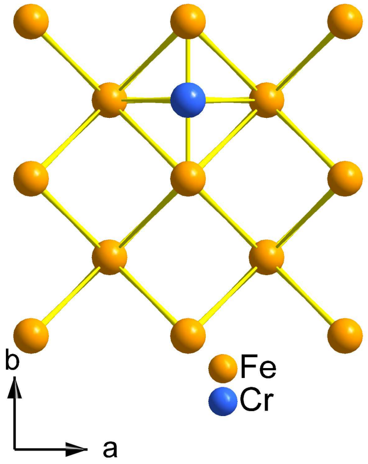

Figure 1. Schematic view of unrelaxed Fe with 12.5% of interstitial Cr.

The optimization of the supercell has been performed by employing a density functional theory (DFT) implemented using linearized augmented plane wave (LAPW) method in the full potential Wien2k code [15]. It is known that the Cr impurities perturb the antiferromagnetic surrounding of Fe_α which is obtained in the substitutional alloys. Therefore, to study the effect of spin polarization, two different relaxation approaches have been employed. In the first approach, the atomic optimal positions were calculated in the local density approximation (LDA) on a 2×2×5 $\boldsymbol{k}$-points grid. In the second procedure, to consider the states with different spin orientations, we have optimized the structure by employing a local spin density appromixation (LSDA). The results of both methods of structural relaxation are represented in Fig. 2.

The central feature which is commonly present after performing both LDA and spin polarized-optimization is the clusterization of the sublattice of iron atoms. In the LDA-picture (Fig. 2(a)), the clusterization leads to the formation of a high-symmetry network. In the $(x,\, y)$ planes, this network consists of Fe_6-octahedra in the middle of the edges of tetragonal unit cell which are connected to the nearest neighbouring iron octahedra by the Fe-Cr bonds. It is worth noting that despite the significant displacements of iron atoms, the net electric polarization of the cell is zero due to high structural symmetry C4/m remaining after the relaxation. The formation energy of the relaxed Fe_8Cr configuration can be calculated as $E_f^{\rm LDA} = E_{\rm tot}({\rm Fe_8Cr}) - 8E_{\rm tot}({\rm Fe}) - E_{\rm tot}({\rm Cr})$, where the last two terms are the total energies of bulk bcc $\rm Fe_\alpha$ and Cr respectively. For the bulk $\rm Fe_\alpha$ we used the energy value obtained in the ferromagnetic state, whereas the total energy of bulk Cr has been calculated for a nonmagnetic state. Using the total energies obtained from the LDA we find that $E_f^{\rm LDA} = 2.37$ eV.

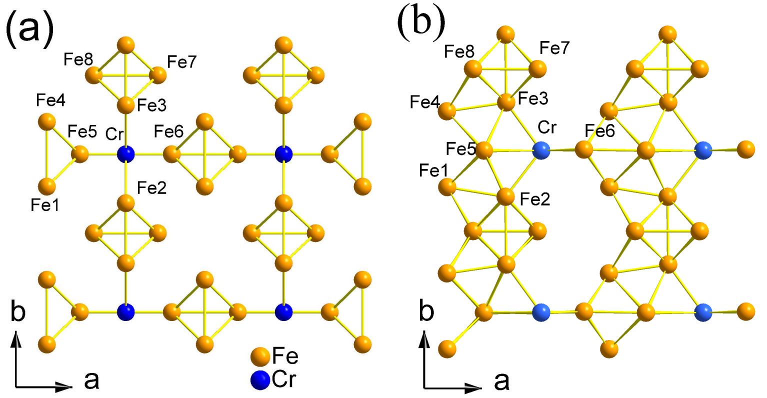

Figure 2. Relaxed structure of Fe with 12.5% of Cr: (a) LDA calculations and (b) spin-polarized LSDA calculations.

In our LDA-calculations, the stuctural relaxation leads to the local magnetic moment for Cr $\mu_{Cr} = -1.19\mu_B$, which is of the opposite sign to the moments of Fe atoms. Furthermore, we obtain that the most distant from Cr iron atoms have the bulk moment 2.5 μ_B. In the close vicinity of Cr, the magnetic moments of Fe are substantially suppressed to the values 1.19 μ_B. As a result, the appearing magnetic spatial pattern is strongly inhomogeneous and contains the antiferromagnetic regions in the vicinity of Cr separated by ferromagnetically ordered Fe atoms. The obtained significant suppression of the Fe moments close to Cr is in contrast to the substitutional Fe-Cr alloys for which our LSDA calculations give almost homogeneous values of all Fe moments in the range 2.72-2.87 μ_B whereas for the magnetic moment of Cr we obtain $\mu_{Cr} = -2.84$ μ_B.

In distinction to the LDA-results, the LSDA optimization produces a completely new ordered structural pattern shown in Fig. 2(b). This pattern is characterized by the chains of $\rm Fe_6$- octahedra alternatively tilted around y direction by the angle $\delta = \pm 8.88$ deg. The obtained chains are paralelly arranged along the x axis with the distance about 4 Å between the Fe atoms in the neighbouring chains, and are connected to each other by Fe-Cr bonds of the length 2.4 Å. The local antiferromagnetic ordering is characterized by the enhanced magnetic moments $\mu_{Cr} = -1.64$ μ_B and $\mu_{Fe} = 1.74$ μ_B of the neighbouring Fe atoms. The magnetic moments of more distant iron atoms have the values around 2.79 μ_B which is close to values found in substitutional alloys.

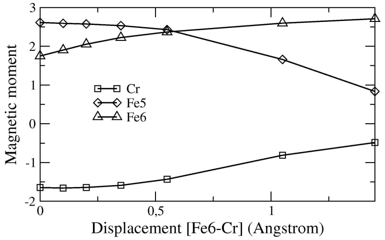

Figure 3. Local magnetic moments of the atoms in Fe5-Cr-Fe6 triad versus the displacement Δ=[Fe6-Cr]-[Fe6-Cr]^0 of Cr along the (100) axis. Here [Fe6-Cr]^0 is the equilibrium distance between Fe6 and Cr.

As compared to the tetragonal structure of the LDA-optimized system, the chain- like structure of the LSDA-relaxed supercell is characterized by substantially lower crystal symmetry. The formation energy of the LSDA-relaxed $\rm Fe_8Cr$ configuration $E_f^{\rm LSDA} = E_{\rm tot}({\rm Fe_8Cr}) - 8E_{\rm tot}({\rm Fe}) - E_{\rm tot}({\rm Cr}) = -2.2$ eV which is well below the energy $E_f^{\rm LDA}$ of the formation of the LDA- configurations. We can also calculate the energy gain due to the structural relaxation by the LSDA approach $\Delta E^{\rm LSDA} = E_f^{unrlx} - E_f^{\rm LSDA} = 4.05$ eV which demonstrates a high stability of the relaxed spin-polarized structure.

Furthermore, due to significant displacements of Fe atoms, the resulted net electric polarization is nonzero, similarly to ferroelectric systems. Due to the coexistence of magnetic and ferroelectric polarization, the appeared structure can be characterized as multiferroic. What can be a possible reason for simultaneous formation of static magnetic and electric dipoles in the interstitial Fe-Cr alloy?

The answer to this question is closely connected to the magnetic exchange energy which depends on the interatomic distance. To see how the atomic displacements affect the magnetic properties of surrounding atoms, in Fig. 3 we show the local moments of Cr and of two nearest nearest neighboring Fe as a function of the Cr displacement $\Delta = x({\rm Fe6}) - x({\rm Cr})$ between Fe5 and Fe6 along the x axis. The increase of Δ leads to significant changes of $\mu_{\rm Cr}$ from -1.65 μ_B to the value about

-0.4 μ_B. On the other hand, the larger Δ leads to the shortening of the [Fe5-Cr] distance and consequently to the reduced μ_{Fe5} which implies a tendency for suppression and possible reorientation of the magnetic moment of Fe5. Moreover, the larger [Cr-Fe6] distance leads to the increase of μ_{Fe6} from 1.7 μ_B to the values about 2.5 – 2.6 μ_B close to its bulk ferromagnetic value 5/2 μ_B.

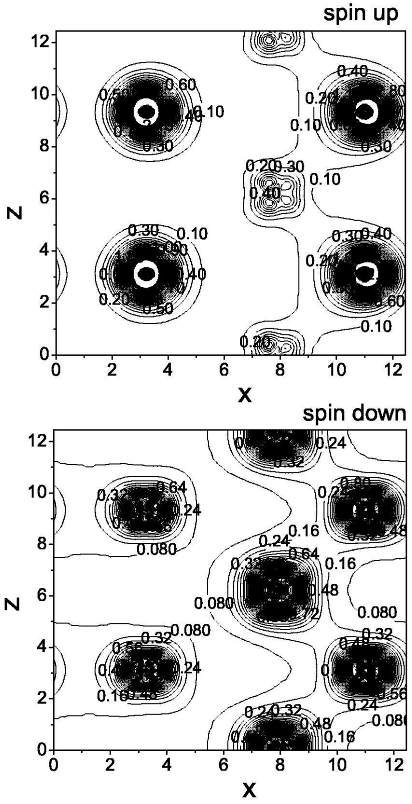

Figure 4. Contours of electron density maps in the (x, z)-plane (y/b = 0.25) obtained by integration of electron states in the energy window E between −3 eV below the Fermi level and the Fermi level. The results obtained by the structural optimization using the LSDA approximation.

Like in other multiferroics, the obtained magnetoelectric coupling is related to the anisotropy of the magnetic moments, the effect produced by spin frustration [2]. To analyze the exchange energies, we performed a mapping of our LDA-results on an Ising- type pseudospin model where J_{kl} denotes the exchange constant between kth and lth atoms in the unit cell. In the proximity of Cr, we obtain the following values for the exchange couplings: $J_{56} = -0.16$ eV, $J_{95} = 0.12$ eV, $J_{96} = 0.12$ eV, where the index "9" denote the Cr atom in Fig. 2(b), and the indices "5" and "6" indicate Fe5 and Fe6 atoms respectively. The results clearly show a spin frustration in the Fe5-Cr-Fe6 triad which appears due to implantation of Cr with its tendency for antiferromagnetic order into the ferromagnetic surrounding of iron atoms.

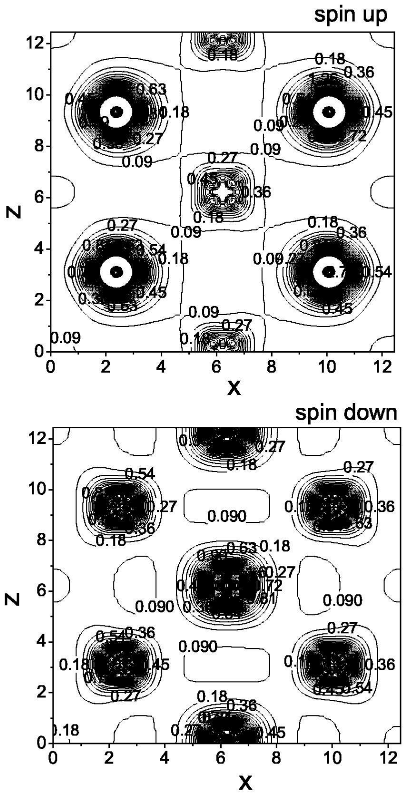

Figure 5. Contours of electron density maps in the (x, z)-plane (y/b = 0.25) calculated by the integration of electron states in the energy window E between −3 eV below the Fermi level and the Fermi level. The LSDA results obtained in the initially LDA-relaxed structure.

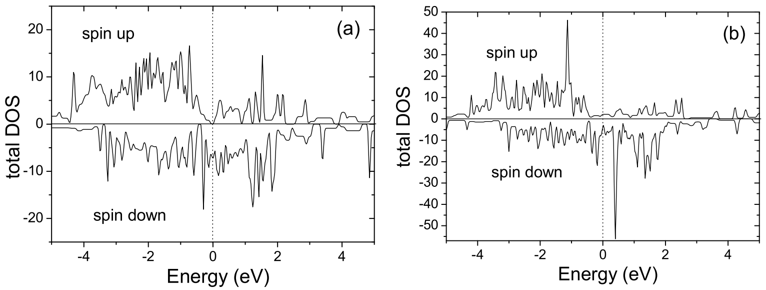

Figure 6. Total density of states for structures optimized using (a) LDA approximation and (b) spin-polarized LSDA approach.

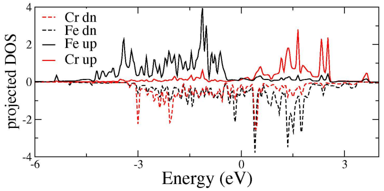

Figure 7. Density of states for Cr and neighbouring Fe2 in the relaxed ferrite structure with 12.5% of interstitial Cr.

In the optimization procedure, the obtained coupling between the magnetic and structural degrees of freedom (magnetoelectric effect) will inevitably produce a structure where a modified magnetic polarization is connected to the atomic displacements and corresponds to the minimum of the total energy. In view of this, we can note that the neglecting magnetoelectric coupling does not allow to achieve a full relaxation in this type of alloys. This conclusion is also supported by Fig. 2(a) where a completely different unpolarized structure appears from the relaxation solely of the structural degrees of freedom.

In the electrically polarized relaxed structure, the valence $3d$ electronic density contours strongly differ for the spin-up and spin-down states (see Fig. 4). The plots show the $3d$ spin-up states of Fe highly occupied by electrons whereas the electron concentration on Cr spin up states is much lower. The opposite effect with high electron occupation of Cr and lower electron density on Fe is obtained for the spin-down electrons. The observed in this case chain-like structures Fe-Cr in the z-direction result in strong hybridization between the intra-chain $3d$ spin-down orbitals of Fe and Cr. The last feature leads to the spatial charge redistribution and

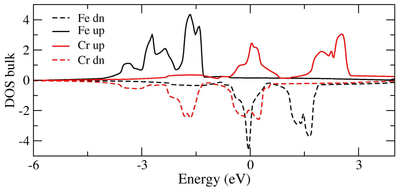

Figure 8. Total densities of states for bulk Cr and Fe.

to higher charge densities on the bonds between spin-down Cr and Fe.

Fig. 5 shows for a comparison the contours calculated for LDA-optimized structure which was later used for the LSDA electronic structure calculations. Similarly to the results in Fig. 4, the electron density on Fe and Cr orbitals and on the bonds between Cr and Fe is much lower than the charge density on the spin-down contours. Moreover, one can clearly see that in the LSDA-optimized system, the structural optimization produces substantial voids with very low charge density, one such a void can be identified between the chain of Fe-octahedra and the Fe atoms located in the left part of the relaxed cell structure. As can be seen in Fig. 4, the voids are almost free from the electrons and can be considered as channels for the diffusion of light atoms like H, Li or N.

For the obtained relaxed structures, the density of states is characterized by strong suppression of the majority spin-up DOS near the Fermi level (Fig. 6(b)). In contrast, the minority spin-down DOS exhibit significant values at the Fermi level. The similar features are also found in the LDA-optimized systems (Fig. 6(a)) which demonstrates a prevailing tendency for suppression of the metallic state of electrons with one spin direction. Such a suppression is typically observed in half-metallic systems where the electric current is conducted by electrons with the same direction of spin [16]. In the considered structure, the local antiferromagnetism in the vicinity of Cr leads to the lower spin-up density of states for Fe atoms which are coupled to the poorly occupied spin-up Cr states (Fig. 7). In contrast to the bulk Fe, the bulk Cr spin-up density of states exhibits well defined finite peak at the Fermi level shown in Fig. 8. Consequently, in the Fe-Cr alloy, the finite spin-up DOS of Cr is suppressed at the Fermi level due to the luck of hybridized spin-up states of Fe. We also note that both Fe and Cr bulk spin-down states have high DOS near the Fermi level which is the reason for the high minority DOS in the Fe-Cr alloy observed in Fig. 7.

The obtained half-metallic-like properties of interstitial alloys Fe-Cr allow us to suggest these materials as possible candidates for spin polarizers in the spintronic devices. Although the present work considers only one particular case of the interstitial alloy with 12.5% of Cr which is periodically located and ordered in the Fe_α lattice, the half-metallicity seems to be a robust feature which appears in the system due to the local antiferromagnetic surrounding near the Cr atom. Another question related to the stability of such an interstitial alloy is how other kinds of atomic impurities can influence the obtained half-metallic properties. In the structurally relaxed system, the location of the light impurity atoms like N or Li is expected to be mainly restricted to the voids. As a consequence, the diffusion of the impurities should be considered in the context of possible diffusion paths within void-based channels in Fe_α.

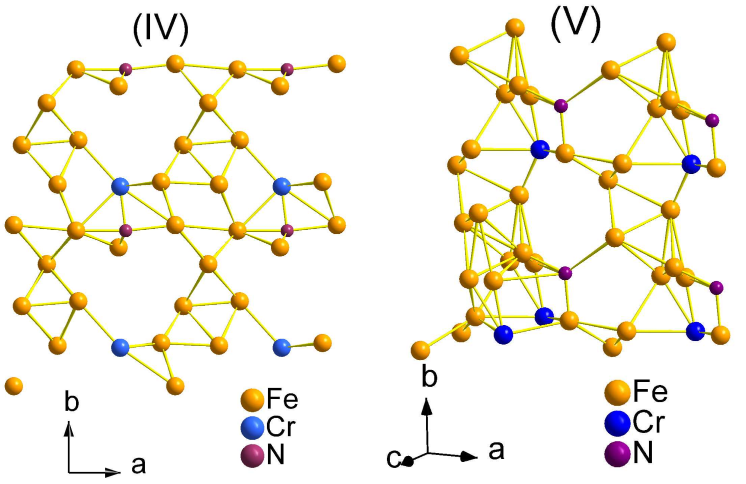

Figure 9. Two different cases of structure relaxation due to the migration of N in the channel of the optimized crystal cell of Fe-Cr. The top picture represents the location of N on the boundary of the cell with $z = 0$, and in the bottom structure N at $z = 0.5c$ is located inside the unit cell.

3. Diffusion paths of N in interstitial alloys Fe_α-Cr

It is worth to note that the voids produced by the atomic relaxation form well defined diffusion channels along the (001) direction. In the two different configurations shown in Fig. 9, such a channel contains one atom of N. The top picture presents an example of N on the boundary surface of the cubic cell with $z_\mathrm{N} = 0$, whereas the bottom picture demonstrates a configuration with N ($z_\mathrm{N} = 0.5c$) located inside the cell. As a consequence, the diffision paths of N contain two stages: (i) the intracell stage with the migration of N within the cell and (ii) the intercell stage which combines the diffusion of N near the boundaries of the cells and the crossing of these boundaries.

To study the diffusion process in the channel, we consider first the relaxed structure of Fe-Cr alloy without any iclusion of N. In this structure with the formed (001)-channels, we choose an interstitial position for N inside the channel (position (I) indicated in Fig. 10) and perform full LSDA optimization of the generated Fe-Cr-N trinary alloy. In this way, by continuous relaxation of the surrounding due to the migration of N, we can study the diffusion paths and the activation energies for the migration of N atoms inside the alloy. The results of the full relaxation of the surrounding are presented in Fig. 9 in the two snapshots of the cell atomic structure. In these pictures, modifications of the position of N due to the migration is accompanied by additional changes of the surrounding atomic Fe- und Cr- coordinates.

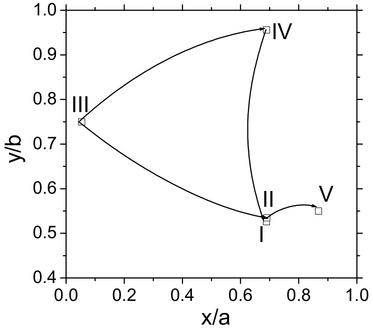

Figure 10. Schematic paths of the migration of N inside the conducting channel. Here the positions I-IV on the face $z = 0$ of the unit cell correspond to the surface migration of N. The position V ($z = 0.5c$) is located inside the unit cell and is related to the diffusion of N inside the structure.

An example of a diffusion path formed by connections of the positions I-II-III- IV-V is shown in projection on the (x, y)-plane in Fig. 10. To consider the full diffusion mechanism, two types of positions for N have been selected: (i) the positions I-IV on the boundary $z = 0$ and (ii) the internal position V with $z = 0.5c$ inside the unit cell. As a consequence, the possible migration paths include: (a) the surface migration I-IV where N

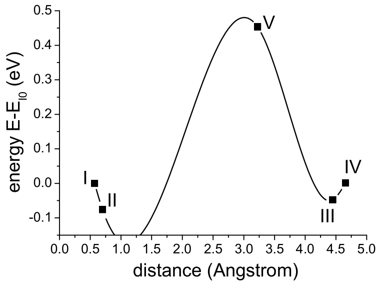

Figure 11. Total energy of the system versus the distance from N to the initial position (I) of N near the Fe5-Cr-Fe6 triad.

remains localized on the boundary between the neighbouring unit cells; (b) the dissufion of N inside the cell (I, II)-V which in fact corresponds to the motion of N inside the channel. Using the described above procedure of the structural relaxation for each considered fixed position (k) (k=I-V) for N, we have calculated the energy costs $\Delta E_{kl} = E_k - E_l$ for the migration of N. In the definition of ΔE_{kl}, E_k is the total energy of the relaxed system with N fixed in the position k. The results in Fig. 11 clearly show the presence of the energy barriers ΔE_{II-V} and ΔE_{III-V} which must be overcome in the course of the N migration inside the channel. With the lowest barrier $\Delta E_{III-V} \approx 0.5$ eV, the diffusion coefficient in the Arrhenius form is given by $D_{\rm N} = \nu_{\rm N} \exp(-\Delta E_{III-V}/RT)$ and strongly depends on temperature and the transition rate $\nu_{\rm N}$. For instance, at room temperature $T = 300$ K, one needs the values of the rate factor $\nu_{\rm N} \sim 5 \times 10^2$ cm·s^{-1} to obtain a non-negligible diffusion coefficient $D_N = 0.2 \times 10^{-5}$cm·s^{-1} of N impurities in the channel of Fe-Cr alloy.

The question which arise due to inclusion of N into Fe-Cr alloy is how the N impurities modify the electronic properties this system. Fig. 12 presents the density of states of the relaxed structures Fe-Cr-N corresponding to the surface configuration (II) and to the internal configuration (V) of N. In both cases, the main effects is related to the electron transfer from Cr and Fe to the $2p$ orbitals of N which leads to the electron depletion on $3d$ orbitals of Fe and Cr. As a consequence, the half-netallic gap in the majority spin-up states becomes larger and approaches the values about 0.2 eV. This effect is found for the structure (II) as well as for all similar structures with surface location of N. For the internal configuration (V), the gap is suppressed and almost disappears due to the increase of the distances from the internally located N to the atoms Fe and Cr of the neighbouring chains.

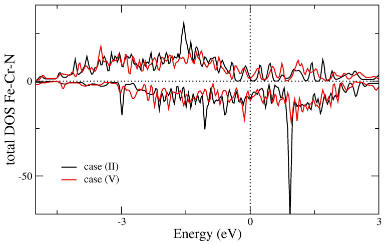

Figure 12. Total density of states for structure FeCrN with 12% of Cr and 12% of N located in three different position of the structure optimized by the use of a spin-polarized LSDA approach.

4. Conclusion

We have shown that the full atomic relaxation of the bulk ferrite with 12.5concentration of interstitial Cr stabilizes a new chain-like structure of lower symmetry. In this structure, the monoatomic Cr in the edges of ferrite bcc cells lead to the local atomic distortions and result in a formation of parallel chains of alternatively tilted Fe6-ochahedra which are connected by interchain Fe-Cr bonds. The energy gain caused by such a structural relaxation approaches 4.05 eV which makes this type of monoatomic interstitial Cr highly stable and energetically favourable. In the investigations of the magnetic state of the new relaxed structures, we have obtained a local antiferromagnetic order in the close proximity of Cr atoms, whereas more distant Fe atoms are coupled ferromagnetically. In the chain-like structure, the atomic distortions result in the formation of a new metallic and multiferroic state with the properties close to half-metallic. The static electric polarization appears due to inhomogeneous spatial disoribution of magnetic moments due to their fructration by Cr impurities. We suggest to consider the generated intersitial alloys as perspective candidates for future applications of in spintronic and multifunctional devices.

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