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Magnetic behavior of clusters $\mathrm{Fe}_1/\mathrm{V}_N$ ($N \leq 144$) embedded in a Fe matrix

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Abstract. The magnetic properties of clusters $\mathrm{Fe}_1/\mathrm{V}_N$ ($N \leq 144$) in bulk Fe are determined by using a realistic *spd*-band Hubbard-like model. The spin density distribution is calculated self-consistently in the unrestricted Hartree-Fock approximation. The local magnetic moments $\mu(i)$ and the densities of electronic states $\rho_i(\varepsilon)$ are obtained at various atoms i of clusters and of the surrounding matrix. The Fe atoms couple antiferromagnetically with the V atoms. In most cases the Fe moments close to the V atoms are reduced, [e.g., $\mu(6) = 1.82\mu_B$ in $\mathrm{Fe}_1/\mathrm{V}_{50}$]. The magnetic order into the clusters is not well defined, in some cases the magnetic order in the V atoms is antiferromagnetic, in another cases the magnetic order is ferromagnetic and in other cases the both magnetic arrangements coexist.

PACS. 75.50.Bb Fe and its alloys – 75.75.+a Magnetic properties of nanostructures

1 Introduction

Atomic clusters have physical and chemical properties different from the bulk and have opened new prospects in the development of material science. The ability to produce experimentally systems in the nanometer range and the unexpected properties observed, make nanoclusters a very attractive field of research. Therefore clusters are the candidates to realize highly functional materials that cannot be achieved even by the present day state of art technology [1]. In particular magnetic nanostructures are expected to revolutionize the magnetic information industry [2].

Most of the attention is focused on the use of transition metals of the Fe group whose electronic and magnetic properties are very sensitive to the structural and chemical environment of the atoms, this behavior has motivated the production and experimental study of a large variety of complex magnetic materials involving transition metals in different geometrical arrangements, trilayers [3,4], superlattices [5], multilayers [6]. In the scientific literature exit recent experimental [7] and theoretical studies [8] about the importance of orbital contributions to the magnetic moments of nanostructured systems of transition metals. Among the future implications of these studies, it would be relevant to investigate the role of electron correlations beyond the mean field theory, since they may affect the localized versus delocalized characters odd the d electron states.

The Fe-V systems are one of the most studied, because to the fact that the hybridizations between V and a strong magnetic element like Fe could induce magnetic ordering in V; neutron-diffraction studies [9], first-principles calculations [10] and self-consistent tight-binding calculations [11] displayed sizeable magnetization on V atoms. Also Korringa-Kohn-Rostoker Green-function studies for V impurities in Fe [12,13] and absorbate V atoms on Fe substrate [14].

Fe/V interfaces can be produced easily using different techniques like molecular beam epitaxy or sputtering [15]. These systems are quite interesting, not only from the fundamental point of view but also for their possible applications [16]. The analysis of these Fe/V interfaces is delicate; theoretical and experimental works concerning the same sample have led sometimes to contradictory results. Even among the different theoretical calculations as well as among the existing experimental studies one can see important discrepancies, but from all these studies on Fe/V interfaces, it is clear that there exist an induced magnetization at V interface antiferromagnetically coupled with the Fe surrounding atoms, and a decrease in the magnetization at the Fe interface atoms.

There has been a great interest on studying how the interface will affect the properties of thin magnetic films, such as coercivity, magnetic domain structure, magnetization reversal and magnetoresistance, these magnetic

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properties greatly affect the applications of thin magnetic films in the magnetic recording industry, as well as other applications in magnetoelectronics. In addition to interface effects many other factors, such as film thickness, composition, crystalline structure of the magnetic film, magnetic domain distribution and correlations contribute to the magnetic energy and determine the magnetization mechanism of a film. These are very important factors that cannot be neglected in practice. However, in order to distinguish which factor dominates, a more detailed study is necessary.

From a fundamental point of view, one of the most interesting features of such systems is the existence of strong long range interlayer magnetic coupling between two successive ferromagnetic layers separated by nonmagnetic or antiferromagnetic spacers, that is, the magnetization of two successive Fe layers were aligned antiparallel. Therefore, the free Fe-V bimetallic systems, particularly $\mathrm{Fe}_1/\mathrm{V}_N/\mathrm{Fe}_M$ clusters, represent a very interesting problem for its study.

In this paper we study in detail the interdependence of the cluster inclusion and the magnetic interactions between Fe and V atoms. The geometrical structure consists of one Fe atom surrounded by N V-atoms ($N \leq 144$) located in bcc onion like shells, and embedded in a Fe matrix; the V atoms are located as substitutional impurities.

This specific problem has been chosen not only for its potential technological relevance, but for the rich magnetic behavior of Fe/V interfaces [17–19]. The competition between the paramagnetism of V and the ferromagnetism of the Fe matrix offers particularly interesting physical situations for studying the interplay between the magnetic properties of clusters and those of the environment. Moreover, the study of finite embedded clusters stresses the local aspects of the magnetic interactions between ferromagnetic and non-magnetic materials, putting aside the translational symmetry of extended interfaces, therefore, from the perspective of interface magnetism, this work provides complementary information to investigations on layered systems.

Besides, our results can be used in the study of magnetic properties of free Fe-V bimetallic clusters, these systems are particularly interesting because the interface does not compite with the Fe matrix and will fix the role of the matrix on the magnetic behavior into the cluster.

The remainder of the paper is organized as follows. In next section we present the details on how the electronic calculation was performed, which parameters were used and we give specific information on the geometry of the clusters, other applications of this method may be found in references [20–22]. The results obtained are presented and discussed in Section 3. Finally, in Section 4 we present the conclusions of this work.

2 Model

The magnetic properties at $T = 0$ are determined by solving a realistic *spd*-band model Hamiltonian including intra-atomic Coulomb interactions in the unrestricted Hartree-Fock approximation. In the usual notation the Hamiltonian is given by

$$H = \sum_{i\alpha\sigma} \varepsilon_{i\alpha\sigma} \hat{n}_{i\alpha\sigma} + \sum_{\alpha\beta\sigma} \sum_{i\neq j} t_{ij}^{\alpha\beta} \hat{c}_{i\alpha\sigma}^{\dagger} \hat{c}_{j\beta\sigma} \tag{1}$$

where i refers to the atomic sites, α and β to the orbitals (s, p, d), and σ to the spin. $\hat{c}_{i\alpha\sigma}^{\dagger}$ and $\hat{c}_{j\beta\sigma}$ are the creation and annihilation operators, respectively. $t_{ij}^{\alpha\beta}$ are the hopping integrals between sites i and j and orbitals α and β, and the environment dependent energy levels $\varepsilon_{i\alpha\sigma}$ are given by

$$\varepsilon_{i\alpha\sigma} = \varepsilon_{i\alpha}^{0} + \sum_{\beta} \left(U_{\alpha\beta} \Delta\nu_{i\beta} - \sigma \frac{J_{\alpha\beta}}{2} \mu_{i\beta} \right) + z_i \Omega_{\alpha} \tag{2}$$

where, $\varepsilon_{i\alpha}^{0}$ stands for the energy level of the orbital α of atom i in the paramagnetic solution of the bulk (e.g., V, or Fe). The second term in equation (1) takes into account the level shifts due to the redistribution of the spin polarizated density and to the resulting intra-atomic Coulomb interactions. $\Delta\nu_{i\beta} = \nu_{i\beta} - \nu_{i\beta}^{0}$, where $\nu_{i\beta} = \langle \hat{n}_{i\beta\uparrow} + \hat{n}_{i\beta\downarrow} \rangle$ is the average electronic occupation of the orbital $i\beta$ and $\nu_{i\beta}^{0}$ the corresponding average occupation in the bulk. $\mu_{i\beta} = \langle \hat{n}_{i\beta\uparrow} - \hat{n}_{i\beta\downarrow} \rangle$ refers to the spin polarization of the orbital $i\beta$. The intra-atomic direct and exhange Coulomb integrals are denoted by $U_{\alpha\beta}$ and $J_{\alpha\beta}$, respectively. Finally, the last term in equation (2) takes into account the environment-dependent energy-level shifts due to nonorthogonality effects [24] and to the crystal-field potential of the neighboring atoms [25], which are approximately proportional to the local coordination number z_i. The average occupations, $\nu_{i\alpha}$ and the local magnetic moments $\mu_{i\alpha}$ at site i are determined self-consistenly by requiring

$$\langle \hat{n}_{i\alpha\sigma} \rangle = \int_{-\infty}^{\varepsilon_F} \rho_{i\alpha\sigma}(\varepsilon) d\varepsilon \tag{3}$$

where $\rho_{i\alpha\sigma}(\varepsilon) = (-1/\pi)\mathrm{Im}G_{i\alpha\sigma,i\alpha\sigma}(\varepsilon)$ refers to the local density of states (LDOS) at the spin-orbital $i\alpha\sigma$. In the case of finite embedded clusters, the Fermi energy ε_F is given by the matrix (in the present case Fe). The local Green's functions are calculated from equations (1, 2) by using the recursion method [26]. The number of levels M of the continued fraction expansion of $G_{i\alpha\sigma,i\alpha\sigma}$ is chosen large enough so that the calculated orbital occupations and magnetic moments are independent of M. All the recursion coefficients are determined exactly without spurious boundary effects. Therefore a large number of atoms, (about 25000−40000) is involved in the real-space expansion.

2.1 Parameters

The parameters used in the calculations are determined as follows. The hopping integrals $t_{ij}^{\alpha\beta}$ between atoms of the same element are fitted to band-structure calculations for the pure elements [27]. The heteronuclear hoppings at

Table 1. Coordination numbers of an atom in shell i located in shell j, for the bcc arrangement. The sublattice for each site is indicated in the first row.

		α	β	α	α	β	α	α	β	α	α	β	β	α	β	α	α	α	β	α	α
No. of Atoms	Shell $i\backslash j$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
1	0	0	8																		
8	1	1	0	3	3	0	1														
6	2	0	4	0	0	4															
12	3	0	2	0	0	4	0	0	2												
24	4	0	0	1	2	0	1	1	0	2	1										
8	5	0	1	0	0	3	0	0	3	0	0	1									
6	6	0	0	0	0	4	0	0	0	0	0	0	4								
24	7	0	0	0	1	0	1	0	0	2	2	0	0	1	0	0	1				
24	8	0	0	0	0	2	0	0	2	0	0	0	2	0	2						
24	9	0	0	0	0	1	0	0	2	0	0	1	1	0	2	0	0	0	1		
8	10	0	0	0	0	0	1	0	0	0	3	0	0	0	0	0	3	0	0	0	1

the clusters-matrix interface are obtained as the geometric average of the corresponding homonuclear hoppings, this procedure has been proved to be a very good approximation in calculations for alloys and multilayers of transition metals [28], and in the study of the magnetic properties of Fe clusters embedded in Cr bulk [23]. In the case of Fe, the d-electron exchange integrals are chosen to yield the proper magnetic moment and exchange splittings in the bulk at $T = 0$, $J_{dd}(\text{Fe}) = 1.05$ eV. For the case of V, $J_{dd} = 0.72$ eV is obtained from local spin-density approximation (LSDA) [29]. Exchange integrals other than J_{dd} are neglected. For simplicity we ignore the differences between s and p integrals (i.e., $U_{ss} = U_{sp} = U_{pp}$ and $U_{sd} = U_{dd}$) and take the ratios between the direct Coulomb Integrals U_{ss}:U_{sd}:U_{dd} from atomic Hartree-Fock calculations [30].

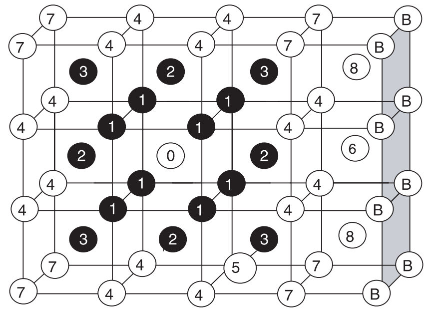

Fig. 1. A cluster with 26 sites belonging to a bcc lattice. The numbers correspond to the nth neighbor shell to the central atom denoted by zero and the sites belonging to V cluster are shown as black circles and to the Fe atoms as open circles, the Fe bulk sites are denoted by B, we show only few atoms, due to the symmetry the other atoms can be inferred.

2.2 Geometrical aspects

The systems studied here consist of a central site (denoted as 0) and its neighbor shells, onion-like shells, around it in a bcc array. A shell is a set of atoms located at the same distance from the central site and with the same number type of neighbors. The lattice structure is illustrated in Figure 1. Here the numbers label the atomic sites in the different shells i. The first shell, sites 1 in Figure 1, contains 8 first nearest neighbors (NN), located at the vertices of the cube. The next shell of neighbors (sites 2) has 6 atoms at a distance $1.15d_{NN}$ (d_{NN} is the nearest neighbor distance), and are located on the square face sites of the next generation cube. Shell 3 is formed by 12 atoms at a distance $1.52d_{NN}$ from the center, and so on.

In Table 1 we list some of the geometrical characteristics of this bcc array, we consider 20 shells in our system. In the first column we give the number of atoms in the shell. The shell numbers are given in the second column and the first row. In the rest of the table we give the number of first neighbors of an atom i-shell located in j-shell. For example, an atom in shell 5 has 1 nearest neighbor in shell 1, 3 in shell 4, 3 in shell 7, and 1 in shell 10. Since we are dealing with a bcc lattice, the total number of NN must sum eight, the shells are ordered as the radius increase. In the present work the central site is a Fe atom. The spacer between the central atom and the Fe matrix is formed by V shell. The number of shells depends on the total number of V atoms. The V atoms are located as substitutional impurities in the Fe bcc lattice, occupying the full shell of neighbors, we neglect the lattice relaxations around the impurities by fixing the neighboring host atoms at the Fe lattice positions. It has been shown that in Fe-V systems like V_N atomic clusters embedded in bulk Fe [11] and in Fe_nV_m superlattices [33], the magnetic order into the V atoms is mainly antiferromagnetic (AF); therefore it is important to note that in order to describe the antiferromagnetism in the V inclusions, it is necessary to subdivide the inclusion lattice sites into sublattices. Thus, the sites that belong to the sublattice α are those in shells 2, 3, 5, 6, 8, 9, etc., and to the β sublattice are the sites in shells 1, 4, 7, 10, 11, etc. In Figure 1 we show a cluster with 26 atoms.

Table 2. Local magnetic moments results for the various cases studied here. For each cluster there are 3 rows; in the first row we give the kind of atoms in each shell, Fe or V, in the second row the value of the local magnetic moment $\mu(i)$ in atomic sites of shell i, and in the third row the number of NN V(Fe) atoms to Fe(V) in shell i.

$N\backslash i$	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19
	Fe	V	Fe	Fe	Fe	Fe	Fe													
8	1.04	−1.28	1.82	1.99	2.23	2.07	2.26													
	8V	8Fe	4V	2V	8Fe	1V	8Fe													
	Fe	V	V	Fe	Fe	Fe	Fe	Fe												
14	0.71	−0.30	−0.31	2.09	2.13	2.14	2.24	2.25												
	8V	5Fe	4 Fe	2V	1V	1V	8Fe	8Fe												
	Fe	V	V	V	Fe	Fe	Fe	Fe	Fe											
26	−0.77	0.27	−0.45	−1.06	1.93	2.05	2.22	2.15	2.29											
	8V	2Fe	4Fe	6Fe	3V	1V	8Fe	1V	8Fe											
	Fe	V	V	V	V	Fe	Fe	Fe	Fe	Fe										
50	0.23	−0.007	0.17	0.02	−0.63	1.94	1.83	2.19	2.04	2.16	2.25									
	8V	2Fe	8V	2Fe	5Fe	4V	4V	1V	2V	1V	8 Fe									
	Fe	V	V	V	V	V	Fe	Fe	Fe	Fe	Fe	Fe								
58	0.22	0.03	0.15	0.019	−0.42	−0.20	1.86	2.13	2.11	2.17	2.18	2.29								
	8V	1Fe	8V	2Fe	4Fe	4Fe	4V	2V	2V	1V	1V	8Fe								
	Fe	V	V	V	V	V	V	Fe	Fe	Fe	Fe	Fe	Fe							
64	0.05	0.08	0.09	−0.03	−0.19	−0.41	−0.58	2.10	2.08	2.19	2.19	2.14	2.30							
	8V	1Fe	8V	2Fe	3Fe	4Fe	4Fe	2V	2V	1V	1V	1V	8Fe							
	Fe	V	V	V	V	V	V	V	Fe	Fe	Fe	Fe	Fe	Fe	Fe	Fe				
88	0.07	−0.03	0.10	0.18	−0.20	0.09	−0.50	−0.94	1.90	1.97	2.15	2.25	2.11	2.32	2.17	2.26				
	8V	1Fe	8V	8V	3Fe	1Fe	4Fe	6Fe	4V	3V	1V	1V	2V	8Fe	8Fe	1V				
	Fe	V	V	V	V	V	V	V	V	Fe	Fe	Fe	Fe	Fe	Fe	Fe				
112	−0.06	0.02	0.07	0.03	0.05	−0.02	−0.39	−0.30	−0.41	1.94	2.12	1.94	2.12	2.20	2.19	2.26				
	8V	1Fe	8V	8V	1Fe	1Fe	4Fe	4Fe	4Fe	3V	1V	3V	2V	1V	8Fe	1V				
	Fe	V	V	V	V	V	V	V	V	V	Fe	Fe	Fe	Fe	Fe	Fe	Fe	Fe		
136	−0.12	0.02	−0.03	−0.001	0.15	−0.003	−0.41	0.007	−0.46	−0.69	1.94	1.85	2.12	2.10	2.21	2.41	2.31	2.18		
	8V	1Fe	8V	8V	8V	1Fe	4Fe	2Fe	4Fe	5Fe	4V	4V	2V	2V	8Fe	1V	8Fe	1V		
	Fe	V	V	V	V	V	V	V	V	V	V	Fe	Fe	Fe	Fe	Fe	Fe	Fe	Fe	Fe
144	0.10	0.01	−0.02	−0.0005	0.14	0.04	−0.41	−0.004	−0.47	−0.42	−0.24	1.88	2.14	2.10	2.39	2.11	2.33	2.16	2.29	2.13
	8V	1Fe	8V	8V	8V	8V	4Fe	2Fe	4Fe	4Fe	4Fe	4V	2V	2V	8Fe	2V	8Fe	1V	8Fe	1V

3 Results and discussion

In all the cases studied local charge neutrality is imposed at each site i. The self-consistent calculations involved the Fe atom, all the V cluster atoms and the Fe matrix atoms at least up to the fifth shell away from the interface between the cluster and the matrix atoms. Beyond this shell the spin-density is taken to be the same as in pure Fe. Due to the characteristics of the system studied here, there are two interfaces, one between the Fe central site and V atoms of the spacer, and the other one between the boundary atoms of the V spacer and the Fe matrix. In the first case, as can be seen from Table 1 and Figure 1, the central site coordinates only with the eight V atoms of the second shell for any number of V atoms. On the other hand, the cluster-matrix interface is not uniquely defined and the interface cluster-matrix becomes more complex as the number of V atoms increases. For example, for $N = 8$ the interface is between the eight V atoms in shell 1 and the 26 Fe atoms in shells 3, 4 and 6, whereas for $N = 26$ the interface is between the 26 V atoms in shells 1, 2 and 3 and the 56 Fe atoms in shells 4, 5 and 7.

Starting with $N = 50$ some V shells are totally surrounded by V atoms; the 6 V atoms in shell 2 have that property; the same occurs for the 18 V atoms in shells 2 and 3 for $N = 88$. One has to notice further that the sites in shells 2 and 3 belong to the same sublattice β and are not nearest neighbors (NN). Similarly the 50 atoms in shells 2, 3, 4 and 5 in V_{144} cluster form a compact core of V atoms surrounded only by V atoms.

Results for the local magnetic moments for the cases studied here are given in Table 2. For each cluster there are three rows, in the first row we give the kind of atoms in each shell, Fe or V; in the second row the value of the magnetic moment $\mu(i)$ of atoms in sites of shell i, and in the third row the number of NN V(Fe) atoms to Fe(V) in

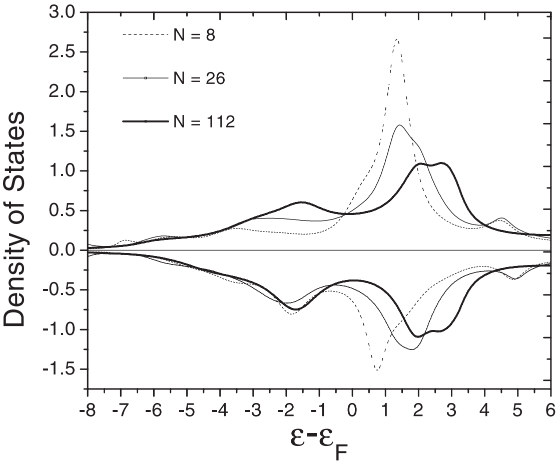

Fig. 2. Cluster average of the local density of states (DOS) at V_N clusters. Positive (negative) values correspond to up (down) spins. Energies are referred to Fermi energy. The dashed line correspond to $N = 8$, the thin solid line is for $N = 26$ and the thick solid line correspond to $N = 112$.

shell i. We recall that the total number of NN is eight. The various cluster sizes were obtained by adding a full shell of V atoms to the previous cluster. The largest cluster consists of the central Fe atom surrounded by the 10 V neighbor shells. To understand the results it is important to note that the V piece of lattice has to be subdivided into two sublattices. Assuming that the Fe central atom is in α-site, the shells that belong to the same sublattice are 2, 3, 5, 6, 8 and 9. On the other hand, the shells 1, 4, 7, 10 and 11 belong to the β sublattice.

In Table 2, we see how the self-consistent solution for the magnetic moments at the various non equivalent sites change as a function of N. We notice that the sign of the interaction as well as the magnitude of the local moments depend strongly on the size of the inclusion. This reflects the high dependence of the solutions on the geometrical environment.

We found that magnetic interaction in the cluster-matrix interface is AF, according to experimental studies [15,18,34] and theoretical calculations [11,31–33,35]. We show in Figures 2 and 3 the electronic densities of states (DOS) for some particular cases that illustrate the hybridization between the Fe and V electrons. The DOS of Fe bulk is given for the sake of comparison. In the Figure 2 we show the DOS for V_N clusters ($N = 8$, 26 and 112). In all these cases the majority bands correspond to the spin down bands, reflecting the AF coupling with the Fe atoms, all the V atoms located at the cluster-matrix interface give this behavior of these DOS, see Tables 1 and 2. This behavior can be qualitatively understood in terms of the hybridizations between Fe and V orbitals d. In the case of V and other transition metals like Cr, the d orbital energy levels are closer to the Fermi energy ε_F and to the spin-down d levels of Fe than to the spin-up Fe d levels that are below ε_F. Therefore, the down states of V hybridize more strongly with Fe matrix than the V up states. Consequently, V down states are preferentially occupied yielding an AF interface coupling [32]. In contrast, if V and Fe moments are parallel the opposite trend would hold [12]. This AF coupling rules the magnetic arrangement of the cluster. Due to the geometry of the bcc lattice there is frustration and not all the boundary atoms and the cluster atoms can fulfill an AF arrangement.

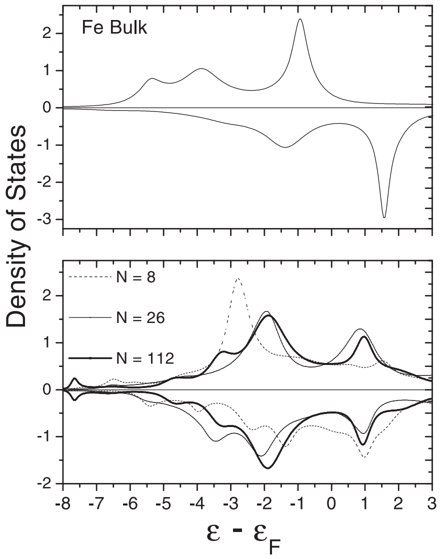

Fig. 3. The electronic local density of states (DOS) for Fe central atom (down panel), for Fe_1/V_8 (dashed line), Fe_1/V_{26} (thin solid line) and Fe_1/V_{112} (thick solid line), in the upper panel we show the DOS for Fe bulk.

In Figure 3, the DOS for Fe bulk and for the Fe central atom in V_8, V_{26} and V_{112} are shown. In all the cases, for $\varepsilon > \varepsilon_F$ are localized states in the up band that are not present in $\rho_\uparrow(\varepsilon)$ in the DOS for Fe bulk, these states increase with N, we can notice that for $\varepsilon < \varepsilon_F$, the number of down electrons is also larger than the up electrons, producing a negative magnetic moment, but these inequality decreases when N increase. These two effects [reduction of $\rho_\uparrow(\varepsilon)$ below ε_F and increase of $\rho_\uparrow(\varepsilon)$ above ε_F] contribute to the lessening of the Fe atom central magnetic moment.

From Tables 1 and 2, we can distinguish two type of frustrated bonds, one into the cluster atoms, and other one at the interface atoms (Fe-V), i.e., the magnetic coupling between them (V-V, or Fe-V) is not AF. For $N = 26$, 50 and 136 are the cases with no frustrated bonds between V atoms, whereas the cases in which there are no frustrated bonds at the interface cluster-matrix are those for $N = 8$, 14, 64 and 144.

These frustrated bonds play an important role in the value of the $\mu(i)$, in sites with a large number of frustrated bonds, the self-consistent solutions yield very small values from the magnetic moments. For example $\mu(1)$ and $\mu(3)$ for $N = 58$; $\mu(2)$ for $N = 64$; $\mu(4)$ for $N = 112$ and $\mu(7)$ for $N = 144$, on the other hand, in situations where the atomic sites coordinate with a small number of frustrated bonds, the magnetic moments $\mu(i)$ have a significative value. For example, $\mu(1)$ and $\mu(2)$ for $N = 14$ and $\mu(1)$ for $N = 26$.

From Table 2, we can notice that the behavior of the local magnetic moments for V atoms, is not monotonic, for $N = 14$, the atomic sites 1 and 2 are located at the interface, both sites prefer the AF coupling with the matrix, and can not satisfy an AF coupling between them, they present a frustrated bond and their respective $\mu(i)$ are reduced, we notice that both sites have almost the same local environment, therefore the value of the local magnetic moments no present a significative difference.

This same behavior is found in V_{26}, all the V atoms are located at the interface, here the magnetic coupling between the NN V atoms is AF, as was mentioned above the atomic sites 2 and 3 are located at the same sublattice and they are not NN atoms, in this case exist a frustrated bond between the site 1(V) and the site 5(Fe), the magnetic coupling is F, therefore $\mu(1)$ takes the smaller value in this case. This behavior, is found in V_{58} and V_{64}; in the first case, the $\mu(i)$ that are aligned parallel, are $\mu(1)$ with $\mu(2)$ and $\mu(3)$, whereas for the last case, the parallel alignment is between $\mu(1)$ with $\mu(2)$ and $\mu(3)$ with $\mu(4)$, for $N = 112$ we found several V atoms whose $\mu(i)$ are aligned parallel, between them and with the Fe matrix atoms, for example $\mu_V(4)$ is parallel with $\mu_V(2)$, $\mu_V(3)$ and with $\mu_{Fe}(9)$, for V_{144} the magnetic frustrations are present only into the V cluster, for example, $\mu_V(7)$ is aligned parallel with $\mu_V(3)$, $\mu_V(8)$ and with $\mu_V(9)$.

Into V atoms, the magnetic frustrations are present when the AF order into the cluster shells is not compatible with the alignment of the NN moments at the interface.

Respect to the magnetic moments of the Fe atoms, we found that the local magnetic moment of the Fe central atom is strongly reduced when the number of V atoms in the spacer is increased. In Fe_1/V_8, this reduction is approximately 53% of the value of the magnetization of bulk Fe, and the magnetization in the V atoms is the largest value, because the hybridizations with the shifted Fe d levels yield a narrower V d band than in V bulk and since the d electron exchange splitting is larger at the Fe atoms than in V bulk, this same behavior is found in $\mu(3)$ for V_{26}.

For $N > 8$, the reduction in $\mu(0)$ can be explained in terms of the smaller exchange splitting at the V atoms surrounding the Fe atom.

As was mentioned above, this system present frustrations, and the Fe central atom present frustrated bonds with their 8 V NN atoms, because the magnetic coupling is not AF, this behavior is present only for $N = 58$, 64 and 144.

Respect with the value of the local magnetic moments in the Fe atoms located at the cluster-matrix interface, are reduced from 1.3% to 18%, this reduction is due to the presence of V atoms in their NN shell, from the Table 2, we note when the V NN atoms is 4 the $\mu_{Fe}(i)$ present the stronger reduction, and may be interpreted as a frustration effect because these atoms can not satisfy an AF coupling with the V atoms and a F coupling with Fe atoms at the same time, see Table 2 for $\mu_{Fe}(6) = 1.86\mu_B$ in Fe_1/V_{58} and $\mu_{Fe}(10) = 1.94\mu_B$ in Fe_1/V_{136}.

This can be qualitatively understood as the result of hybridizations between Fe d orbitals and the V d orbitals, which increase the effective local d-band width at the Fe atoms of the interface.

These results shown that $\mu_{Fe}(i)$ at the interface are very sensitive to the local environment of atom i.

Our results can be compared qualitatively, as experimentally as theoretically, for example. The magnetic behavior at the interface V-Fe(matrix) atoms, as the F coupling as AF coupling between them, is found in the experimental work of Walker and Hopster, [19], in which they find that the magnetization of the V surface of two monolayers of vanadium aligns ferromagnetically with the substrate and the V layer adjacent to Fe is aligned antiferromagnetically these authors estimated the local magnetic moment of the surface to be less than $0.4\mu_B$, this last result is concording with Fe_1/V_{14}, see Table 2; this oscillatory behavior is reported by Fuchs, Totland and Landolt [18], they established a reduction in the Fe magnetization about 20%, which is in good qualitative agreement with our results. The AF coupling at the interface Fe-V was found in a recent experiment about ulrathin Fe on V(100) [34] and the V atoms at the interface displayed a magnetic moment of $-0.8\mu_B$, this value is concording with our calculated local magnetic moments μ_V, see Table 2.

Theoretically, the magnetic coupling at the interface Fe-V atoms had been reported for several systems, for example ab initio calculations of Fe overlayers on V [35], for all the cases studied they found an AF coupling between Fe-V atoms. In V overlayers on Fe(100) [33], the oscillatory behavior is found for 3 monolayers of V, the surface present a magnetic moment with value of $= 0.35\mu_B$ and has a F coupling with the Fe substrate.

The magnetic frustrations had been found in free bcc V clusters, giving low values for the local magnetic moments in the atomic sites with frustrated bonds [36], therefore is interesting to extend the present study to systems of free Fe-V bimetallic clusters.

4 Conclusions

The interface effects on the magnetic moments in the system Fe_1/V_N embedded in a Fe matrix have been studied by solving a realistic *spd*-band model Hamiltonian in the unrestricted Hartree-Fock approximation. The competition between the ferromagnetic order of the matrix and the tendency of V to antiferromagnetic-like order results in a remarkable dependence of the magnetic solutions on size and environment. The main conclusions are summarized as follows.

(a) The magnitude of the $\mu(i)$ of V atoms have a significative value by the presence of Fe atoms in their NN shell [e.g., $|\mu(1)| = 1.28\mu_B$ in V_8, $|\mu(3)| = 1.06\mu_B$ in V_{26} and $|\mu(7)| = 0.94\mu_B$ in V_{88}]. On the other hand, the $\mu(i)$ of Fe atoms close to the cluster, usually tend to be reduced [e.g., $\mu(2) = 1.82\mu_B$ in V_8 and $\mu(11) = 1.88\mu_B$ in V_{144}], and the ferromagnetic order of the boundary Fe atoms is never altered by the presence of the V atoms.

(b) The magnetic moments of the boundary Fe atoms, $\mu_{Fe}(i)$, are very sensitive to the local environment of atom i, when the number of V atoms is 4, the $\mu_{Fe}(i)$ present the lowest value. Into the V atoms, magnetic frustrations are present when the antiferromagnetic order into the cluster shells is not compatible with the antiparallel alignment of the NN moments at the interface. These frustrations lead to small values of $\mu(i)$ in the cluster [e.g., $\mu(3) = 0.02\mu_B$ in V_{50}; $\mu(1) = 0.08\mu_B$ in V_{64}].

(c) In the V_N cluster, the magnetic order is depending of N, for V_{14} the magnetic order is ferromagnetic, and for V_{26} and V_{50} the magnetic order is antiferromagnetic, whereas for $N \geq 58$ the antiferromagnetic order and the ferromagnetic order coexist into the V_N cluster [e.g. for V_{144}, $\mu_V(4)$ is aligned parallel with $\mu_V(5)$ and antiparallel with $\mu_V(6)$].

(d) The value of the magnetic moment of the central Fe atom $\mu_{Fe}(0)$ is decreasing with N. The magnetic coupling between the Fe central atom and its first 8 V NN atoms is ferromagnetic for $N = 58$, 64 and 144, this behavior was found in an experimental work of V overlayers on Fe substrate [19]. This magnetic coupling is also found in the boundary atoms [e.g., $\mu_V(1)$ with $\mu_{Fe}(5)$ in V_{26} and $\mu_V(3)$ with $\mu_{Fe}(7)$ for V_{50}].

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