

Magnetic properties of Fe/V nanostructures

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The decrease of Fe magnetic moments in slow cooled bulk bcc Fe-V alloys and existence of the “magnetically dead” Fe layers on V(110) substrate are explained in terms of a compositional order and magnetic disorder. Self-consistent calculations of the magnetic moments distribution for the ordered and disordered Fe-V alloys and thin Fe films on V(110) with intermixing of the atoms at the interface are performed in the framework of vector periodic Anderson model. The calculations show the sharp decrease of the average magnetic moments for the ordered FeV equiatomic compound in the CsCl structure and for the alloys containing the small paramagnetically ordered Fe clusters in V matrix in comparison with the disordered bulk alloys of the same concentration. We found that the decrease of the magnetic moments also takes place in thin ordered FeV films as well as in isolated paramagnetically ordered Fe clusters evaporated on the V(110) substrate. Intermixing of Fe and V atoms at the interface significantly affects the magnetic properties of the films. The magnetization of the Fe/V(110) films with ideally smooth interface decreases after introduction of the disorder by layer-by-layer random intermixing procedure. On the contrary, in the FeV compound film the intermixing gives rise to the magnetization.

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I. INTRODUCTION

The effect of chemical ordering on the magnetic properties of the Fe-V alloys is the subject of many investigations. Vanadium, being a nonmagnetic transition metal in its bulk bcc state, reveals a magnetic moment in an environment of the magnetic atoms¹ as well as in the geometries with a reduced coordination number.² In surroundings of Fe atoms, the vanadium atom acquires a magnetic moment, which usually appears to be antiparallel to the Fe moments, whereas the Fe magnetic moment decreases gradually with the increase of the number of V atoms in the nearest surroundings and disappears completely in V neighborhood.³ The influence of vanadium content on the magnetic properties of bulk Fe-V alloys was extensively discussed (see Ref. 4–7). It was shown⁸ that in the experimental temperature-composition phase diagram the iron-vanadium system forms a continuous series of chemically disordered bcc solutions except a region around the equiatomic composition, where the alloys tend to form the chemically ordered FeV compound with CsCl structure.⁹ By means of magnetic measurement, Nevitt and Aldred⁵ found that the average magnetic moments of the alloys decrease gradually with the vanadium concentration. The ordered and disordered Fe-V equiatomic samples have different average moments per Fe atom: i.e., $0.4 \mu_B$ for the ordered FeV compound and $0.6 \mu_B$ for the disordered alloy. The average moment at about $0.7 \mu_B$ was obtained for the random substitutional Fe-V alloys of equiatomic composition by Johnson *et al.*¹⁰ within the first principles calculations using spin-polarized self-consistent Korringa-Kohn-Rostoker coherent-potential approximation (KKR-CPA) method. The calculations showed the decrease of the moments with vanadium concentration. The moments vanish when the concentration becomes greater than 70 at. % of V in agreement with

the Nevitt and Aldred experiment.⁵ Neutron-diffraction studies by Chandross and Shoemaker¹¹ on the ordered FeV equiatomic compound displayed a lower value of the average magnetic moment at about $0.35 \mu_B$ per Fe atom. First-principles band calculations by Moruzzi and Marcus⁷ turned out in a good agreement with the neutron-diffraction measurements. It was shown⁴ that for the disordered alloys the average magnetic moment falls down to zero with the increase of the vanadium concentration to 77 at. %. In recent investigations by the dc magnetization, Mössbauer spectroscopy, and x-ray diffraction on the quenched Fe-V alloys by Krause *et al.*¹² the zero magnetization was also found to be in agreement with the Nevitt and Aldred results⁵ (at 70 at. % of V). A strong dependence of the magnetic properties on the sample preparation technique was found. In particular, the slow cooled samples showed a reduction of the saturation magnetization in the full concentration range with the zero value at about 40 at. % of vanadium. Mirebeau *et al.*¹³ found that a similar heat treatment of the samples results in an enhancement of a short-range order. The shift of Mössbauer spectra towards lower values of the hyperfine field was partially explained by this short-range order induced by the V-V repulsion.¹² The main reason for a gradual decrease of the saturation magnetization and hyperfine splitting was supposed to be in the degradation of the Fe magnetic moments. Krause *et al.*¹² excluded the presence of appreciable amount of a paramagnetic phase and magnetic disorder. Indeed, the microscopy investigations of Sanchez *et al.*¹⁴ showed that the heat treatment led to the increase of the ordered FeV phase of CsCl-type in the disordered alloys.

From the experimental investigations discussed above one can make a conclusion about a cause-effect relation between the degradation of the Fe atomic magnetic moment in the slow cooled alloys and the simultaneous increase of the

short-range order. However, the effect of the ordered equiatomic FeV phase on the magnetic properties of the heat treated alloys was not studied. The correlation between the magnetic properties of the alloys and the amount of the ordered FeV phase needs both an experimental and theoretical study.

Another fascinating point is an effect of surfaces and interfaces on the electronic and magnetic properties of the Fe/V system in its thin film form. This influence was recently investigated within semiempirical and *ab initio* approaches^{15–20} for ideally sharp or stepped interfaces. It turns out that calculated values of the total magnetic moment of the Fe/V multilayers somewhat deviate from the experiments of Refs. 21 and 22. At the same time the different approaches predict the similar magnetic profiles, i.e., magnetic moments of the Fe atoms are reduced and the V atoms show noticeable magnetic moment at the interface. These features were also reproduced within the periodic Anderson model (PAM) for the multilayered structures.²³ The PAM parameters were adjusted for a consistency with the density of states and magnetic profiles of *ab initio* calculations for structures with an ideally sharp interface. In the real structures, however, the alloying at the interfaces always exists and may cause some discrepancy between calculations and experiments. Therefore an ordered alloying at the interface was supposed²⁴ to explain the existence of the “magnetically dead” Fe layers,²⁵ i.e., the fact that the V(110) film covered with the iron of about 3 monolayers (MLs) thick does not exhibit any magnetization. The authors of Ref. 24 performed calculations with the scalar-relativistic version of the TB-LMTO method. The overlayers on the V(110) substrate were modeled by the ordered FeV equiatomic compound for thicknesses up to 6 MLs (the largest overlayer is equivalent to 3 MLs of the pure Fe), and by the monolayers of pure Fe for the higher coverages. The results of the calculations are in a good agreement with the experimental data of Ref. 25 for the coverages more than 4 MLs of Fe but show a small deviation from the experiment for the smaller coverages (at about $0.5 \mu_B$ per Fe atom instead of the experimental zero value). It was supposed in Ref. 24 that the discrepancy could be explained by the disorder of Fe and V at the interface but no proofs were given.

In this paper we consider the effect of compositional ordering and magnetic disordering on the Fe magnetic moments in the modeled objects of Fe/V system. The Fe-V bulk 3D alloys and Fe/V films with reduced dimensionality are studied within a unified approach. We model the bulk Fe-V alloys in the whole concentration range with the ordered and disordered compositional structures as well as the structures with small ferromagnetic clusters in the V matrix. In films, we study the effect of interface intermixing of the FeV equiatomic compound with V(110) substrate as well as the presence of isolated Fe islands on the top to clarify the origin of “magnetically dead” Fe layers. Magnetic moments distribution is calculated in the framework of PAM taking into account noncollinear orientation of the magnetic moments at the sites for all of the considered in Refs. 26 and 27 cases.

II. THE MODEL

Periodic Anderson model was shown to be effective in studying Fe/Cr multilayers with a large number of atoms in

the supercell.^{28,29} Self-consistent numerical calculations for more than 1500 nonequivalent atomic sites turn out to be complete in a reasonable time using a modification of zero and poles method for the determination of the mass operator and Green functions poles. Such method reduces the integration time of the density of *d*-electron states in a computational process. The numerical results for the Fe/Cr systems obtained in the framework of PAM are in a reasonable agreement with *ab initio*¹⁵ and semiempirical³⁰ approaches and are successfully used in the interpretation of the Mössbauer experiments.^{31,32}

PAM assumes the existence of two bands: quasilocalized *d* electrons and itinerant *s* electrons. The *s-d* interaction on a site is presupposed to be stronger than *d-s-d* interaction of *d* electrons on the different sites. In this case, one should construct the resonant *d* states of a finite width Γ due to *s-d* interaction and then introduce an electron hopping between the different sites. The hopping integral includes a contribution of direct *d-d* transition between the atoms as well as contributions of the *d-s-d* transition via the conductivity band. A Coulomb repulsion of *d* electrons on a site is taken into account in Hartree-Fock approximation. The theory involves a limited set of parameters: $(E_{di} - \varepsilon_F)/\Gamma$ determines the position of the *d* level at *i*th site relative to the Fermi level ε_F , U_i/Γ is the Coulomb repulsion on the site, and V_{ij}/Γ is the *d* electrons hopping between the nearest neighbors.

In PAM there are two approaches: collinear, where only parallel and antiparallel orientations of the magnetic moments are taken into consideration,²⁶ and noncollinear with an arbitrary orientation of the magnetic moments relative to a global *z* axis.^{27,33} In the noncollinear approach, the polar angles θ_i and φ_i determine the direction of the moment relative to the global quantization axis. In this case, after Hartree-Fock approximation in the PAM Hamiltonian, the hopping on a site with spin inversion arises together with the intersite hopping without change of the spin projection.

The calculation of the vector distribution of the magnetic moments starts from the initial state, preliminarily obtained for the modeled object in the collinear approximation. The initial angles φ_i are assigned zero at every site. The initial angles θ_i are taken either zero or π in accordance with the collinear decision and changed on $\pi/2$ at some sites as a disturbance to deviate starting configuration from the collinear ground state. Then a self-consistent *d* electrons number and magnetic moment are calculated for a slight variation of θ_i at every site, and a state with a minimal energy is accepted for the next iteration.^{34,35} The obtained self-consistent solution is used as an initial state in the procedure for the variation of both angles θ_i and φ_i with the deviation of the later one on $\pi/2$ at some sites. Generally this procedure may guarantee a convergence only to the local configurational minimum of the energy. The energy of the finally obtained noncollinear state is compared with the energy of the initial collinear state to evaluate which of the states is actually preferred.

III. MAGNETIC PROPERTIES OF BULK Fe/V ALLOYS

A. Model parameters

First, we have to determine the parameters of PAM for Fe and V. An estimation of the parameters for transition metals

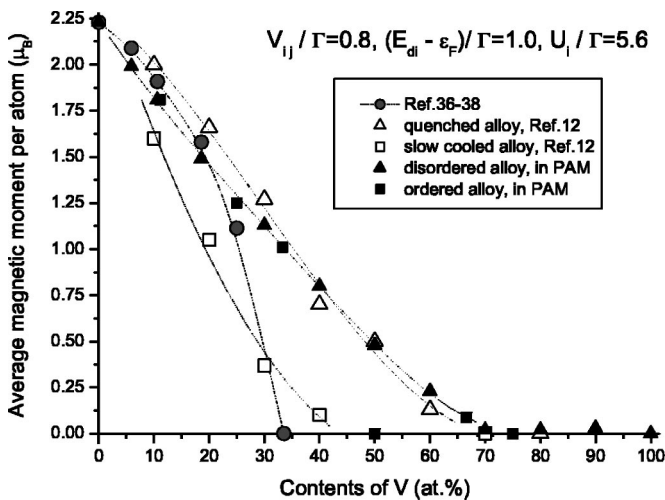


FIG. 1. Average magnetic moment per atom on the V contents. The data depicted as the grey circles are taken from Refs. 37–39; the open triangles and squares stand for the quenched and slow cooled alloys obtained in Ref. 12. The solid triangles and squares correspond to the moments for the modeled quenched and ordered alloys calculated in PAM with the following parameters: $V_{VV}/\Gamma=0.8$, $(E_{dV}-\epsilon_F)/\Gamma=1.0$, and $U_V/\Gamma=5.6$. The lines are guides to the eye.

and alloys has been made by Moriya³⁶ on the basis of the band structure. However, these values give only rough idea of their magnitude and one has to choose the values so that to get reasonable agreement with the various experimental data. Thus, the Fe atoms parameters are taken to reproduce the magnetic moments of the bulk iron:²⁶ $V_{FeFe}/\Gamma=0.9$, $U_{Fe}/\Gamma=13.0$, $(E_{dFe}-\epsilon_F)/\Gamma=-11.5$. The parameters of vanadium are chosen to reproduce the magnetization of the bulk bcc Fe-V. The data on saturation magnetization for the Fe-V alloys with different concentration of vanadium are taken from the Ref. 37 (see Fig. 1, grey circles). One can see a gradual decrease of the average magnetic moment per atom from $2.09 \mu_B$ to $1.58 \mu_B$ in the V concentration range from 5.9 at. % of V to 18.6 at. %. Collins and Low³⁸ showed that in the Fe-V alloy with 1 at. % of V the magnetic moment at a V atom is about $-0.9 \mu_B$. The moments of the Fe atoms located nearest to the V atom are 8% less than the value of $+2.2 \mu_B$ of the pure bulk iron, whereas the moment of the iron atoms located as far as 4 \AA away from the V atom is greater than in the bulk. In the concentration range of 30–60 % of V the solid solution and the intermetallic compound FeV trends toward a coexistence that affects the magnetic properties of the alloys. It was shown in Ref. 39 that a slow cooled alloy demonstrates a zero magnetization at 33.5% of V. Recently Krause *et al.*¹² performed thorough study of the preparation technique effect on the saturation magnetization of Fe-V alloys. The samples in the entire range of concentrations were prepared by melting under high vacuum, then quenched or slow cooled. All samples revealed exclusively the bcc structure. The average magnetic moments for the quenched (open triangles) and slow cooled alloys (open squares) are depicted in Fig. 1. One can see that the average magnetic moments of the slow cooled samples are significantly lower than for the quenched ones. Based on these

facts, the PAM parameters for vanadium are fitted in order to recover the followings conditions: the zero magnetization of the pure V, the value of the magnetic moment on a V atom in the dilute alloy with 1% of V, and the average magnetic moments data for the quenched alloys in the concentration range from 10% to 80% of V from the Ref. 12.

To model the atomic structure we assume that the quenched alloys are completely compositionally disordered and simulate the atoms disposition at the bcc sites independently for each layer in (001) plane by a random procedure. The supercell of 6 successive layers with 6×6 sites in each is taken for the self-consistent calculations of magnetic moments distribution. On the edge of the supercell the periodic boundary conditions are used.

A program of successive parameters selection was written to find the model parameters of vanadium, i.e., V_{VV}/Γ , U_V/Γ , and $(E_{dV}-\epsilon_F)/\Gamma$; the d -electron hopping between the nearest V and Fe atoms was taken as $V_{FeV}=(V_{FeFe} \cdot V_{VV})^{1/2}$. For each taken parameter a successive exhaustive search of the other ones was made, and for all sets of parameters the self-consistent calculations of the magnetic moments at the sites of the supercell were performed. The ranges of considered parameters for the fitting were taken as $0.65 \leq V_{VV}/\Gamma \leq 0.95$, $1.5 \leq U_V/\Gamma \leq 6.0$ with step of 0.05, and $-1.75 \leq (E_{dV}-\epsilon_F)/\Gamma \leq 1.0$ with step of 0.25. The best fitting to the values of the average magnetic moments of the quenched alloys with an accuracy not worse than 6% were obtained for the following parameters: $V_{VV}/\Gamma=0.8$, $U_V/\Gamma=5.6$, $(E_{dV}-\epsilon_F)/\Gamma=1.0$ (solid triangles in Fig. 1).

To check the effect of the supercell size on the magnitude of the magnetic moments we increased the number of the atoms in the layer up to 20×20 sites and the number of the layers up to 10 and did not find an essential difference in the magnitude of the moments (greater than 6%) in the whole concentration range.

B. Ordered and mixed alloys

The ordered alloys are modeled for the concentrations of V atoms $1/9$, $1/4$, $1/3$, $1/2$, $2/3$, $3/4$ in the same way as in Ref. 40. The self-consistent calculations performed in PAM show that the average magnetization per atom for these ordered alloys are very close to the value of the disordered ones with the same composition (see Fig. 1, solid squares). The only exception was found for the equiatomic FeV compound with CsCl-type crystallographic structure, where each iron atom has only V atoms in the nearest shell. The ordered FeV compound is nonmagnetic but even a slight disorder gives rise to a spontaneous magnetization. This means that the spontaneous magnetization takes place only if the iron atoms form simply connected chains or domains where every Fe atom has at least one Fe atom in the nearest neighborhood. In the ordered alloys the chains exist when the vanadium concentration is less than $1/2$. In the disordered alloys, however, the domains exist if the Fe content is greater than the percolation threshold,⁴¹ which is equal to 0.24 for the bcc lattice and corresponds to the V concentration of 0.76.

Our calculations for the equiatomic FeV compound show zero magnetic moments both at the vanadium and at the iron

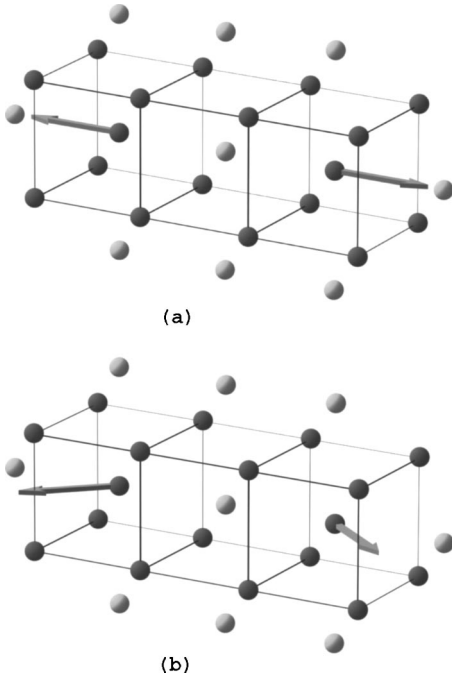


FIG. 2. The Fe clusters in V surroundings with the 180° (a) and 90° (b) orientations of the average magnetic moments. Dark and grey balls correspond to Fe and V atoms, respectively.

atoms. This result is in agreement with calculations of Mirbt *et al.*,³ which displayed zero magnetic moments for the Fe surrounded only by the vanadium atoms. Zero magnetic moments at Fe atoms were found experimentally by means of Mössbauer spectroscopy¹² in the slow cooled Fe-V alloy for V concentration of 40 at. %. The average magnetization per atom was reduced to 0.10 μ_B from 0.70 μ_B in the quenched alloy. Krause *et al.*¹² suggested that the reason of lower magnetization in the slow cooled alloys is in a rise of the short-range order. Therefore, we simulate a structure of isolated bcc Fe clusters consisting of 9 atoms (see Fig. 2). The nearest iron atoms are only in the second shell of the considered Fe cluster. This alloy contains about 44 at. % of vanadium and one may expect that its average magnetization per atom is between the calculated zero value for the equiatomic FeV compound and the experimental one of 0.10 μ_B for the slow cooled alloy with 40 at. % of V (see Fig. 1).

The supercell of $4 \times 2 \times 4$ bcc sites containing 2 separated Fe clusters (see Fig. 2) was modeled for the self-consistent calculations of the magnetic moments distribution. In the collinear approach it was supposed that all the Fe atoms have the same direction of the magnetic moments and the V atoms have the moments orientation opposite to the Fe ones. The values of moments on the central Fe atoms are 2.63 μ_B , on the other Fe atoms are 0.77 μ_B , and on the V atoms are equal to $-0.38 \mu_B$. The average magnetization per atom is obtained of 0.38 μ_B that is much higher than the magnetization given in Ref. 12 for the slow cooled alloy even with 40 at. % of V. Therefore, we suppose that the orientation of the magnetic moments in Fe clusters is noncollinear. For noncollinear calculations all initial angles θ_i on one of the Fe clusters were rotated by π or $\pi/2$ relative to the initial angles of the other

TABLE I. Dependence of the average magnetization M of the supercell per atom and the angle α between the average magnetic moments M_1 and M_2 of the adjacent Fe clusters on the initial angles θ_1 and φ_1 at the sites of the first cluster. The initial angles at the sites of the second cluster equal zero.

θ_1 (deg)	φ_1 (deg)	$M(\mu_B)$	$M_1(\mu_B)$	$M_2(\mu_B)$	α (deg)	$\Delta E/\Gamma$
0	0	0.38	0.58	0.58	0	0
90	90	0.25	0.61	0.61	86	1.47
180	90	0.22	0.66	0.59	92	1.48
90	45	0.14	0.60	0.62	133	1.47
180	180	0.0	0.63	0.63	180	1.47

cluster, and the polar angles φ_i were fixed to zero at all the sites. The obtained noncollinear solution was taken as the initial state with angles φ_i at the same cluster rotated by π , $\pi/2$ or $\pi/4$, and self-consistent calculations were performed.

The calculations show that the magnetic moments inside the Fe clusters are parallel both in the collinear and noncollinear approaches. In the noncollinear approach, the magnetic moment at the central Fe atoms of both clusters are enhanced up to 2.72 μ_B as compare with the collinear approach, and at the cluster edges the magnetic moments of the Fe atoms are reduced to 0.31–0.37 μ_B depending on the initial clusters orientation. The magnetic moments on the V atoms separating the nonparallel clusters are about zero because V moments have to be antiparallel to both of them simultaneously. The average magnetic moments of the adjacent Fe clusters, \mathbf{M}_1 and \mathbf{M}_2 , turn out to be oriented at angle α to each other. The magnitude of α depends on the initial angles at the beginning of the iteration process; the clusters prefer to keep the orientation near to the initial one. The Fe clusters in V surroundings with the 180° and 90° orientations of the average magnetic moments are displayed in Figs. 2(a) and 2(b), where the dark and grey spheres correspond to the Fe and V atoms, respectively. The average magnetization M of the supercell per site, the average magnetic moments M_1 and M_2 of the adjacent Fe clusters, the angles α between \mathbf{M}_1 and \mathbf{M}_2 , and the gain in energy $\Delta E/\Gamma = (E_{col} - E_{ncol})/\Gamma$ are summarized in Table I. The different initial orientations of the magnetic moments at the sites of the adjacent clusters result in the different angles α between the average magnetic moments of the clusters. The value of the average magnetization M of the supercell depends essentially on the mutual orientation of the clusters: it decreases from 0.25 μ_B to zero as α increases from 86° to 180°. One can see that the states with nonparallel clusters orientation are energetically favorable with the energy gain $\Delta E/\Gamma \approx 1.47$. Taken into account the estimation of the model parameters by Moriya³⁶ on the basis of the band structure we assign 1 eV to the level width Γ and obtain the value of the energy gain as 1.47 eV per unit cell or 0.046 eV per atom. So the system avoids a ferromagnetic ordering formation and prefers nonparallel orientation of the clusters when the V atoms have lost their magnetic moments. Thus, as the energy is almost the same for the states with nonparallel moments of the Fe clusters, the magnetic moments of the clusters have no preferable mutual orientation. Therefore, the alloy with the embedded Fe clus-

ters in V matrix may be considered as a superparamagnetic structure.

Our calculations show that the decrease of the average magnetic moments in slow cooled Fe-V alloys with the V content less than 50% can be caused by Fe clusters with the arbitrary orientation of the magnetic moments embedded in the V matrix, as the pure V surroundings prevents an interaction between the Fe atoms. The calculations for more complex structures, containing segregations of the ordered FeV compound and small Fe clusters in the disordered Fe-V alloy, also show a tendency of the average magnetization to decay in the comparison with the disordered alloy. So, we make a conclusion that the slow cooled alloys have rather complicated atomic and magnetic structures with different fractions of the Fe clusters in the vanadium surroundings as well as the ordered FeV compound segregations in the matrix of the disordered alloy. However, the detail experimental investigations of the chemical structure are required.

IV. IRON FILMS ON V(110) SUBSTRATE

In this section, the PAM approach is applied to study the effect of compositional ordering and magnetic disordering on the magnetic properties of Fe films on a V(110) substrate and to clarify the origin of the “magnetically dead” Fe layers.²⁵

First we consider Fe films and interfaces of the same structures as in Ref. 24. The films consist either of 1–6 MLs of the FeV equiatomic compound in the CsCl structure placed on the V(110) substrate, which corresponds to 0.5–3 MLs of the Fe coverage, or of the pure Fe coverage (1–4 MLs) on 6 MLs of the FeV compound.

The self-consistent calculations are performed with the same parameters as for the bulk Fe-V alloys. The supercells of 8×8 sites in each monolayer and different number of layers depending on the coverages are taken for the calculations. The magnetization per Fe atom is found to be zero for all films with FeV compound on the top of V(110). The pure V surroundings suppresses completely the magnetic moment of the Fe atoms not only in the bulk alloy but also for the FeV films on V(110). The results of calculations for the Fe coverage up to 3 MLs are in agreement with Mirbt *et al.*³ calculations, as well as with the polarized neutron reflectometry²⁵ (PNR) and the magneto-optical Kerr effect (MOKE) experiments.⁴² Figure 3 shows the average magnetic moments per Fe atom obtained by PNR experiments²⁵ (solid circles) and the results of our calculations (open circles).

Note that the discussed values of magnetization are perceptibly different in various experimental measurements and in different theoretical approaches for the same compositional structures. For example, theoretical calculations based on the LMTO method²⁴ have given the average magnetic moment of $0.5 \mu_B$ and not zero value obtained in the PAM approach. The MOKE experiments⁴² on the samples with the Fe coverage of about 3 MLs have given the magnetization of $(0.4 \pm 0.4) \mu_B$ instead of zero value in PNR experiments.²⁵ It might be assumed that the variance of the experimental data is due to nonhomogeneity of the samples surface, as an evaporation process can lead to formation of the clusters of

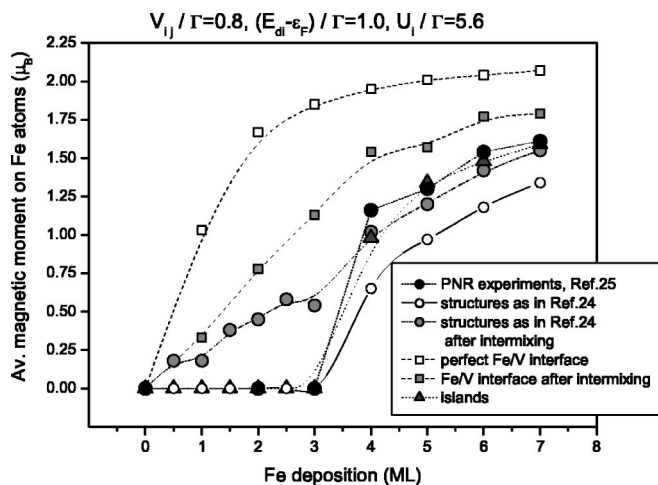


FIG. 3. Average magnetic moment per Fe atom as a function of the Fe deposition thickness on the V(110) substrate. Black circles correspond to the PNR measurements by Nawrath *et al.* (Ref. 25). Open and grey squares correspond to the values obtained in PAM for the pure Fe monolayers at Fe/V(110) interface before and after intermixing. Open and grey circles correspond to the magnetic moments calculated in PAM for the structures of Ref. 24 with the equiatomic FeV compound at the interface before and after intermixing. Grey triangles stand for the structures with the Fe islands on the top of FeV compound layers. The lines are guides to the eye.

one of the components and phases of an ordered alloy. The experimental evidence of such segregation of the ordered alloy was obtained by a means of a scanning tunnel microscopy. It was shown experimentally by Choi *et al.*⁴³ that for the Fe/Cr system the incorporated Fe atoms form the ordered Fe/Cr alloy on the Cr(100) surface. Besides, Fe islands and areas of the disordered Fe/Cr alloy were also observed. These facts could explain the discrepancy between the PNR²⁵ and MOKE⁴² experimental data by the different ratio of the ordered and disordered formations in the Fe films on V(110).

Our calculations performed for the structure with a pure Fe coverage on the top of 6 MLs of the FeV compound give the lower values of the average magnetic moments than in Ref. 24 (see Fig. 3). The reason might be in the perfect interface between the Fe MLs and the FeV compound. Therefore, structures with a random intermixing of atoms at the interface and Fe islands on the top of the films are investigated.

We model a chemical disorder by a random intermixing of the atoms from the neighboring layers using the procedure described in Ref. 44. The layer-by-layer intermixing is made in the assumption that exchange of the atoms takes place only through the surface. We choose a preset fraction of the atoms in the supercell to be intermixed. In every layer this number of atoms are exchanged by a random choice with atoms of the preceding layer in such a way that each chosen atom is exchanged with one of four nearest neighbors taken also randomly. The procedure is carried out layerwise in every pair of the neighboring layers starting from the bottom of the supercell. The intermixing process does not exclude a repeated choice of the lattice sites and thus can return some

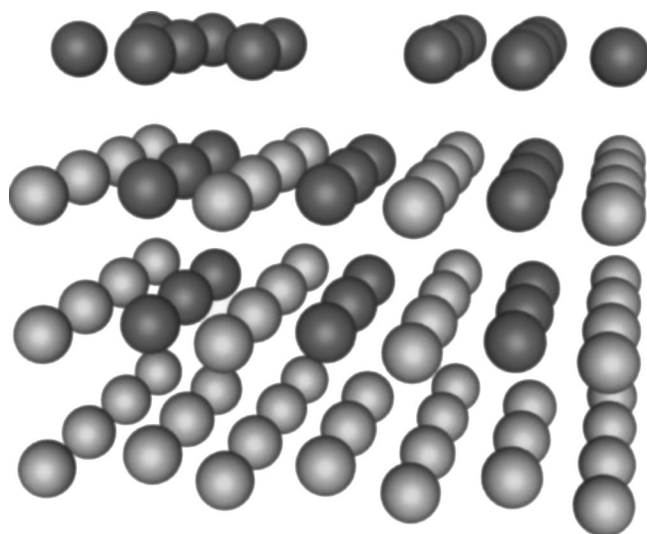


FIG. 4. Model of the surface Fe clusters on the top of V(110) with 2 MLs of the FeV equiatomic compound in the intermediate layers. Dark and grey balls correspond to the Fe and V atoms, respectively.

atoms back into the preceding layer. Such a scheme leads to an asymmetry of the interface: atoms are allowed to flow up several layers but are not permitted move down to the layers below the first interface layer under the considered one.

This procedure is applied to all structures described above with the intermixing fraction of 0.5. The calculations for a small coverage, up to 3 MLs of Fe, result in the values of the average magnetic moment coming up to $0.5 \mu_B$, and for the iron coverage starting from 4 MLs give a good fitting to the experimental data of Ref. 25. These results are shown in Fig. 3 by the grey circles. The intermixing procedure applied to the structures of the pure Fe films (1–7 MLs) on the top of the V(110) substrate with the perfect interface and in absence of the intermediate FeV layer leads to the reduction of the average magnetic moment in comparison with the values before intermixing. The average magnetic moment per Fe atom for the perfect interface and the interface after the intermixing are shown in Fig. 3 by the grey and open squares, respectively.

To consider the effect of small Fe clusters on the magnetic properties of the Fe/V system with reduced dimensionality we reproduce the structure of Ref. 43 for the Fe films on V(110). The modeled samples consist of 5 MLs of pure V at the bottom of the supercell, 1 or 2 MLs of the ordered FeV compound as the intermediate layers, and separated Fe islands, 1–3 MLs thick, on the top. These structures correspond to the Fe coverage from 0.5 to 3 MLs (see Fig. 4). In the numerical calculations we assumed that the magnetic moments at the sites of each iron island are parallel but the mutual orientation of the average moments of two adjacent islands are opposite to each other. In this case, the magnetic moments of the islands compensate each other and self-consistent calculations result in the magnetization of the sample close to zero. The value of the magnetic moment of the central Fe atom in the cluster is enhanced, while the moments of the border Fe atoms are close to the value of the

bulk iron. The dependence of the average magnetic moment per Fe versus the Fe deposition thickness is shown in Fig. 3 with grey triangles.

The calculations show that the thin Fe coverage up to 3 MLs yields a good compliance with the experimental PNR (Ref. 25) data either for the structures with ordered FeV compound or with oppositely oriented Fe islands on the top of the V(110) or FeV compound. The Fe films with perfect Fe/V interface yield the values of the average magnetic moment much lower than experimentally observed by PNR.²⁵ The random intermixing of the atoms applied to the films with the perfect Fe/V interface has not disposed a discrepancy. The intermixing applied to the FeV compound on the top of V(110) leads to the increase of the average magnetic moments up to the values of MOKE experiments⁴² and the LMTO calculations.²³ For the Fe coverage higher than 3 MLs only structures consisting of the FeV compound and pure Fe MLs after intermixing as well as structures with separated islands on the top of the FeV compound give a reasonable agreement with the experiments.

Thus the disorder introduced by the layer-by-layer random intermixing procedure gives rise to the magnetization of the film with the initially nonmagnetic FeV compound on the top of the V(110), in contrast to the pure Fe coverage of the initially perfect Fe/V interface, where the intermixing of atoms decreases the magnetization. The formation of separated Fe islands with the opposite orientation of the average magnetic moments on the top of the ordered FeV compound can significantly reduce the magnetization of the films.

V. CONCLUSION

The calculations show that the periodic Anderson model is very efficient in studying the effect of the compositional ordering and magnetic disordering on the magnetic properties of both bulk Fe-V alloys and the structures with reduced dimensionality. The model parameters of V are evaluated by a fitting procedure for the compliance of the calculated magnetization values with the experimental ones for the disordered alloys in the whole concentration range. It is significant that the same set of parameters can be used to study both bulk alloys and thin films. It is found that the disordered and ordered alloys give the significantly distinct magnetization only for the equiatomic FeV composition. The reduced magnetization of the slow cooled Fe-V alloys is explained by existence of the short-range order modeling as magnetically disordered Fe clusters in vanadium surroundings.

The existence of the “magnetically dead” layers for the Fe films on the V(110) substrate are explained by a trend to formation of the ordered equiatomic FeV compound with magnetically disordered Fe islands on the top. It is found that for all structures studied in Ref. 24, having the FeV compound on the top of V(110) substrate, the average magnetic moment of the films equals zero. The layer-by-layer intermixing of the atoms in the structures with ordered FeV compound leads to the increase of the average magnetization as opposite to the structures with the perfect Fe/V interface, where the intermixing decreases the magnetization. This fact is connected with the suppression of the Fe magnetism by the V matrix.

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