

Modeling of the magnetic properties of the Cr-Fe interface

A. K. Kazansky

Institute of Physics, The University of St. Petersburg, St. Petersburg, 198904, Russia

V. M. Uzdin

Institute of Chemistry, The University of St. Petersburg, Universitetskij pr. 2, St. Petersburg, 198904, Russia

(Received 2 March 1995; revised manuscript received 9 June 1995)

A method of self-consistent determination of magnetic ordering in rough Fe-Cr interfaces is developed. It comprises two basic algorithms. The first algorithm is the EPITAXY routine, which allows one to simulate the structure of the Fe-Cr interfaces. The EPITAXY algorithm works in two variants. One of them creates relatively regular structures while the second variant generates quite irregular interfaces. The second algorithm provides a routine for determination of the magnetic ordering in a spatially inhomogeneous structure. For sets of the interfaces, constructed with the EPITAXY algorithm and comprising 30 configurations, self-consistent calculations of the magnetic properties of the system are performed. This allows us to obtain the average physical quantities of the interface and its dependence on the coverage parameter ζ with a reasonable accuracy. It is shown that low coverages of Cr upon the Fe vicinal surface cause a decrease in the average magnetic moment of the interface iron atoms. The influence of surface roughness on the smoothing of the average magnetic-moment oscillations with surface coverage is demonstrated.

I. INTRODUCTION

The recent development of epitaxial growth technology allows the generation of a great diversity of multilayer samples with well controlled parameters. This has created a new class of materials and phenomena which have become the subject of intensive research. In particular, a number of challenging problems are related to investigation of magnetic properties of superlattices built with magnetic-nonmagnetic bilayers.

One of the appealing multilayer systems consists of Fe-Cr superlattices and sandwiches which exhibit interesting phenomena, for example, giant magnetoresistance^{1,2} and Cr-layer-thickness-dependent oscillations of magnetic coupling between the adjacent Fe layers.^{3,4} A number of experimental studies of these systems have been performed and a substantial influence of interface roughness on the magnetic properties of the superlattices has been revealed. This influence is very important, since rough interfaces are much easier to obtain and are thus more likely to be employed in any future technological applications of multilayers.

Cr-Fe interfaces have been investigated using a range of methods. For example, Unguris, Celotta, and Pierce⁵ generated wedges that exhibit both short and long periods in oscillations of the exchange coupling. These interfaces are not continuous, but consist of a series of steps. In a later paper by the same authors⁶ some magnetic properties of Cr films grown epitaxially on an Fe(100) whisker were investigated as functions of the Cr layer thickness by means of scanning electron microscopy with polarization analysis (SEMPA).

The technique of soft x-ray magnetic dichroism has also been applied⁷ to an Fe/Cr/Fe trilayer epitaxially deposited on the (001) surface of GaAs. It was shown by

this method that Cr atoms exhibit ferromagnetic ordering within each layer and antiferromagnetic ordering with respect to the atoms in the Fe layers. The magnitudes of the magnetic moments on the Cr surface were estimated at $(0.6 \pm 0.2)\mu_B$. Besides this, it was revealed that the total magnetic moment of the sample decreases monotonically during Cr coating. The authors have related this phenomenon to the antiferromagnetic structure of the surface island of Cr atoms on the previously created Cr surface. However, if the coverage parameter ζ is close to 0.25, the experimental data evidence that the decrease of the magnetic moment (while the ζ parameter increases) is more pronounced than the Poisson island model predicts.

Another method of investigation applied to the study of magnetic ordering in Cr/Fe interfaces is spin-resolved core-level photoemission.⁸ The average magnetic moment per one atom for Cr monolayers was estimated in this paper as $(0.5-1)\mu_B$. This experimental work also confirmed the antiferromagnetic coupling of the neighboring Cr and Fe layers, as have spin-polarized electron-energy-loss spectroscopy⁹ and spin-resolved valence-band photoemission studies.

A particularly thorough experimental investigation of the Cr-Fe interface using a magnetometer was performed by Turtur and Bayreuther.¹⁰ They kept track of the dependence of the interface magnetic moment on the coverage parameter ζ . Since the experimental setup allowed the authors to change this parameter continuously, the interfaces obtained were inevitably rough. As a result of this, the regular structure of the antiferromagnetically ordered ideal Cr layers, which was forecast by theoretical calculations of the ideal interfaces, was averaged out. The resultant averaged magnetic patterns depend on the statistical details of the Cr atom distribution in the interface. Description of these correlations is a challenging theoretical problem.

Most of the theoretical investigations were concentrated upon ideal systems. Actually, the theoretical treatment of rough interfaces implies determination of the physical quantities under consideration for a set of randomly constructed interfaces and averaging of the quantities obtained over the ensemble. This requires the development of simple, approximate, but quite accurate, methods of solution of the basic equations which determine these physical quantities. It is to be noted that the conventional accurate methods, for instance, the density-functional method, are overly time consuming and therefore can hardly be effectively applied for a treatment of random systems, although they have been applied^{11,12} for the investigations of ordered layered systems.

The methods with substantial potential for study of complex, spatially nonhomogeneous systems are related to the Hubbard or Anderson models. They are well known to be rather flexible and result in a physically reasonable description of the magnetic properties. Although these models are too complicated to be solved accurately, some quite reliable approximations were formulated within these frameworks. (As an example of application of the Hubbard model to investigation of steplike surfaces see Ref. 13.)

It is worthwhile to note here that there is a number of the model modifications and methods of their approximate investigation. However, we dare to state that such a "pluralism" in the description of complicated phenomenon is quite appropriate to the diversity of the systems under consideration. Of course, all the models and methods of their solution have to be gauged with some rather comprehensive hierarchy of test calculations. These calculations give close but different results for different models. A reasonable theoretical understanding of a phenomenon can be obtained via "voting" by different approaches. We suggest that a model which can be used for our purpose has not necessarily to be a formal consequence of an *ab initio* theory obtained with some elaborate formal mathematics. Preferable for us is a model which, being physically meaningful, has been proven in a set of simple situations.

In this paper we deal with random interfaces and develop an algorithm for *self-consistent* investigation of the magnetic order within the framework of the periodic Anderson model. The method we use here comprises two key algorithms. They are the random modeling of the epitaxial growth process and the iterative solution of the self-consistent system of equations for the occupation of both the spin-polarized states for the atoms at each site. The former routine is described in Sec. II; the latter algorithm is reviewed in Sec. III.

II. THE EPITAXY ALGORITHM

The random modeling of the epitaxy of Fe and Cr atoms on the surface of a vicinal substrate is performed by the EPITAXY algorithm. This algorithm keeps track of the descent of atoms dropped randomly onto the square top of an initially empty prism orthogonal to the (0,0,1) surface of the bcc lattice. [In the bulk the lattice constants a of Fe and Cr almost coincide ($a_{\text{Fe}} = 2.87 \text{ \AA}$;

$a_{\text{Cr}} = 2.88 \text{ \AA}$) and hence one may assume that there is no substantial reconstruction of the lattice at the interface.] In the course of the EPITAXY algorithm performance the prism is gradually filled with atoms. The base of this prism in our calculation comprises 8×8 elementary cells; its height is 18 levels. Outside the prism we periodically repeat its structure.

The lowest level of the prism is initially uniformly covered by Fe atoms. Then, 6×64 Fe atoms are dropped upon the top of the prism. An atom commences its "coasting" from a randomly chosen site at the top. At each step there are four possible positions for the atom at the next level underneath (see Fig. 1). The algorithm chooses the next site using a random routine (with equal probabilities) from the sites which are not filled by atoms nested previously. We consider two different conditions for terminating this atom motion and thus fixing its position in the lattice.

(A) The atom coasts along until all of the four possible next positions are blocked.

(B) If some of the four positions are blocked, the atom

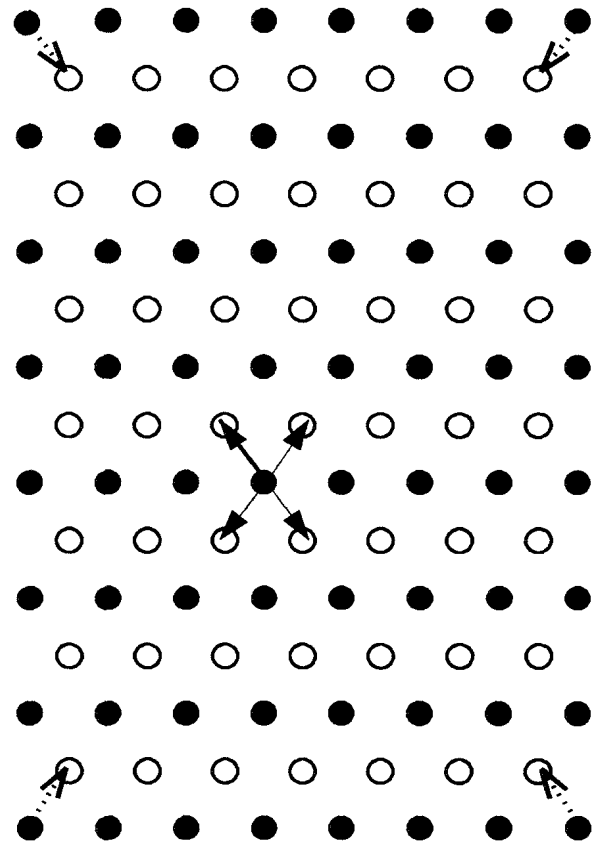


FIG. 1. This snapshot depicts the prism (view from the top) we are dealing with by the EPITAXY algorithm. The solid circles represent the atoms on the level achieved by the atom in the course of its coasting; the empty circles show the positions of the atoms on the level beneath that level. The four possible paths of the atom sliding are shown for the atom inside the prism by the solid arrows and for the atom at the corner of the square area by the dotted arrows. The dotted arrows reflect the periodical recurrence conditions imposed on the configuration.

may either continue its descent with probabilities p_i through each empty site, or it may stop at a particular site with the probability $1 - \sum_i p_i$. The quantities p_i have been taken to depend on the amount of blocked paths.

(i) If three (of the possible four) paths are blocked, the atom either moves to the vacant position with a probability of $\frac{1}{4}$, or is stopped with the probability $\frac{3}{4}$.

(ii) If there are two open paths, the atom either is stopped with the probability $\frac{1}{2}$, or moves to either of the open positions (each with a probability $\frac{1}{4}$).

(iii) If there is only one blocked position, the atom inevitably continues its descent with equal probabilities equal to $\frac{1}{3}$.

Algorithm B produces a rougher interface than algorithm A (see below). If the values of probabilities p_i used are less than above, the densities of the interfaces obtained appear to be unrealistically small.

All the Fe atoms for definiteness are assumed to be spin polarized upward.

After the whole set of Fe atoms is inducted a variable number (determined by the coverage parameter ζ) of chromium atoms is added and their descent determined using either of the above algorithms. In the Cr case it is more convenient to assume that both the spin polarizations are available for these atoms with the probabilities 0.5. It is to be noted here that the final spin polarization of the Fe atoms is quite robust in our study since they strongly prefer to keep ferromagnetic ordering among themselves and the self-consistent solution permanently reproduces this fact. The polarization of the Cr atoms at the interface is more fragile, although, generally,¹⁴ they exhibit antiferromagnetic coupling with respect to the surrounding Fe atoms. Note, however, that for a random interface some of the Cr atoms fail to follow this rule, which causes frustration of their spin polarization. In some configurations of the atoms at the interface, the solution of the self-consistent equations is not always unique. Usually the energies related to these solutions are close so that metastable-configuration solutions also have to be taken into account for description of real samples. (The fact that the solution of a self-consistent problem is not unique is not an artifact of our model, since this phenomenon was revealed in Refs. 13, 15, and 16 as well.) We believe that, taking the initial spin polarization of the Cr atoms by chance, we can somewhat address this very complicated phenomenon.

After the EPITAXY routine has been performed each site inside the prism is either filled by Fe or Cr atoms, or is empty. The parameters and the initial magnetic moments of the atoms are assumed to be equal to their bulk values. The final values of the magnetic moments and electron occupation numbers are then calculated using the self-consistent procedure described in the next section.

As was mentioned above, algorithm B will produce more irregular interfaces than the algorithm A. (For instance, within the A case one obtains the nonporous interface.) We believe that in real interfaces the Cr atoms may penetrate into the Fe layers causing suppression of the magnetic moments of neighboring Fe atoms. (This

statement is sustained by analysis of the total energy of the system calculated within the approach developed previously.¹⁷ We do not intend to present the detailed results here, for the sake of brevity; however, the main conclusion obtained can be formulated as follows: configurations with strong Cr-Fe intermixing are preferable.) Therefore comparison of the results obtained using A and B algorithms should provide an insight into the effect of the interface disorder on the magnetic properties of the interface.

The procedures described above are not perfect enough to be considered as more or less unique, and there is a broad field for improving them to reproduce realistic conditions. It is worthwhile to emphasize that the structure of an interface depends strongly on the details of the epitaxy growth process, which can produce somewhat "irreproducible" results. For instance, by heating of the interface with laser light the surface may be polished. The same result can be achieved via the epitaxy of atoms with substantial tangent velocity, or in the presence of inert gas atoms as well. In the latter case the inert gas atoms may penetrate into the cavities of the Fe interface and fill there the sites vacant for Cr atoms. A drastic influence of the porosity of the Fe substrate on the interface magnetic order is clearly demonstrated in the present work (see Sec. IV). Note that the interface roughness may decrease with time, since there are a number of metastable variants of the interface structure with rather small energy deviations among them. However, we mention these variants only tentatively here, trying to show the substantial arbitrariness of our procedure and attach the attention of experimentalists to the possibility of study of the influence of the experimental environment on magnetic order.

III. THE METHOD OF CALCULATION OF MAGNETIC ORDERING

We assume that the electron spectrum may be described within the two-band approximation, i.e., we deal with the $s(p)$ (itinerant) and d (localized) subsystems. For the localized d electrons we use Wannier- and for the itinerant electrons the Bloch-function representations. The electron system of the d metals is treated within the framework of the Anderson periodic model.

We commence the description of the model with the solitary-impurity case and then generalize it for the present study of the disordered surface alloy. The Hamiltonian of the system in the mean-field approximation reads

$$H = \sum_{i\alpha} E_{i\alpha} \hat{d}_{i\alpha}^\dagger \hat{d}_{i\alpha} + \sum_{\alpha; i \neq j} E_{ij} \hat{d}_{i\alpha}^\dagger \hat{d}_{j\alpha} + \sum_{k\alpha} E_k \hat{c}_{k\alpha}^\dagger \hat{c}_{k\alpha} + \sum_{ki\alpha} V_{ki} \hat{c}_{k\alpha}^\dagger \hat{d}_{i\alpha} + \text{H.c.} \quad (1)$$

Here $\hat{d}_{i\alpha}^\dagger$ ($\hat{d}_{i\alpha}$) and $\hat{c}_{k\alpha}^\dagger$ ($\hat{c}_{k\alpha}$) refer to the creation (annihilation) operators of d electrons with spin α on atomic site i and $s(p)$ electrons with quasimomentum k and spin α , respectively. $E_{i\alpha}$ and E_k are the energies of these electrons. The hopping parameters E_{ij} and s - d hybridization

potential V_{ki} are taken to be spin independent.

The equations for the Green function matrix elements are

$$\sum_j [\omega \delta_{ij} - E_{ij}] G_{j,i'} - \sum_k V_{ik} G_{k,i'} = \delta_{i,i'}, \quad (2)$$

$$[\omega - E_k] G_{k,i} - \sum_j V_{kj} G_{j,i} = 0, \quad (3)$$

$$[\omega - E_i] G_{i,k} - \sum_{k'} V_{ik'} G_{k',k} = 0, \quad (4)$$

$$[\omega - E_k] G_{k,k'} - \sum_j V_{kj} G_{j,k'} = \delta_{k,k'}. \quad (5)$$

This approach implies that the $s(p)$ - d interaction on a site is large compared to $s(p)$ - d interaction between different sites. This allows us to construct first the resonant d states which acquire a width due to the $s(p)$ - d mixing (see Ref. 18). The interaction between different atoms can then be taken into account.

Equations (2) and (3) may be transformed straightforwardly into the following form for the matrix elements $G_{i,i'}$ which account for the d states only:

$$[\omega - E_i] G_{i,i'} - \sum_j V_{ij} G_{j,i'} = \delta_{i,i'}, \quad (6)$$

where the d -electron energies E_i and the hopping integral $V_{i,i'}$ between the localized sites read

$$E_i = E_{i,i} + \sum_k \frac{V_{ik} V_{k,i}}{\omega - E_k}, \quad (7)$$

$$V_{i,i'} = E_{i,i'} + \sum_k \frac{V_{ik} V_{k,i'}}{\omega - E_k}. \quad (8)$$

Thus E_i includes an imaginary part which is determined by the s - d interaction:

$$\Gamma_i = \text{Im} \sum_k \frac{V_{ik} V_{k,i}}{\omega - E_k}. \quad (9)$$

The hopping integral is also renormalized due to this interaction. In the following we take the parameters V and Γ as being independent of site coordinate i .

By iterating Eq. (6), one obtains the following expression for the d -electron Green function:

$$G_{i,i'} = \frac{1}{\omega - E_i} \left[\delta_{i,i'} + \frac{V_{i,i'}}{\omega - E_{i'}} + \sum_{j,l} \frac{V_{ij} V_{j,l} V_{l,i'}}{(\omega - E_j)(\omega - E_l)} + \dots \right]. \quad (10)$$

For the diagonal matrix element we obtain

$$G_{i,i} = (\omega - E_i - \sigma_i)^{-1} \quad (11)$$

where the mass operator σ_i is defined as follows:

$$\sigma_i = \sum_j \frac{V_{ij} V_{j,i}}{\omega - E_j} + \sum_{j,l} \frac{V_{ij} V_{j,l} V_{l,i}}{(\omega - E_j)(\omega - E_l)} + \dots \quad (12)$$

The summation in Eq. (12) proceeds over all transition paths which commence and finish on a given i th site, but

do not move to this site otherwise. To make the system (10)–(12) definite we use the simplest self-consistent condition, which is analogous to the Hartree-Fock approximation, but may be considered as a semiempirical tool beyond the framework of this approximation:

$$E_i^\alpha = E_{0i} + U_i n_i^{-\alpha}. \quad (13)$$

Here $n_i^{-\alpha}$ is the number of d electrons with spin $-\alpha$ on the i th site. The initial energy E_{0i} and the Coulomb integral U_i depend on the type of atoms on the i site. We consider these parameters as phenomenological ones in the spirit of the Fermi-liquid theory. An analogous model was exploited to describe magnetic properties of bulk metals with half-filled d bands and of thin films of these metals.^{19,20} That approach corresponds to inclusion of electron transitions between neighboring sites in the first order of perturbation theory. As an initial approximation, the density of states for a single impurity was used. However, this approach does not permit consideration of complex, nonhomogeneous states, such as clusters of various atoms near the sample surface. Therefore we have used another method, for which it is possible to calculate the mass operator taking into account d - d transitions inside a given number of coordinate spheres.²¹

To calculate the mass function σ_i , let us take a certain set of atoms \mathcal{M}_i , associated with the i th site, and consider only the transitions through the atoms of this set. Then

$$\sigma_i = \sum_{j \in \mathcal{M}_i} V_{ij} S_{j,i}, \quad (14)$$

where $S_{i,j}$ is the contribution from all the paths that start from the i th site and finish at the j th site. We determine the matrix $S_{i,j}$ with the following set of equations:

$$(\omega - E_j) S_{j,i} = V_{j,i} + \sum_{l \in \mathcal{M}_i} V_{j,l} S_{l,i}. \quad (15)$$

It is the gist of our approximation that we have restricted the sum only to the intermediate sites which belong to the set \mathcal{M}_i associated with the i th site.

This method was previously applied²¹ to study magnetic ordering in homogeneous bulk metals with the expanded series of sets \mathcal{M} starting at the first coordination sphere and going up to include the seventh coordination sphere. The results obtained suggest that inclusion of only the first coordination sphere provides a quite good approximation and at present we restrict the set \mathcal{M}_i to the first coordination sphere of the site under consideration. In the case of a bcc lattice one obtains for the σ_i the expression

$$\sigma_i^\alpha = \frac{8V^2}{\omega - E^\alpha}. \quad (16)$$

We have implied in Eq. (16) that the energies E_i^α do not depend on the site i , as is assumed universally for ferro- and paramagnetic order in a homogeneous sample.

The d -electron state occupation numbers are determined with the expression

$$n_i^\alpha = -\frac{1}{\pi} \int d\omega f_T(\omega) \text{Im} G_i^\alpha(\omega - i0), \quad (17)$$

where $f_T(\omega)$ is the conventional Fermi-Dirac function (in what follows we assume the temperature T to be equal to zero).

The set of Eqs. (11)–(17) allows us to calculate the quantities n_i^α and E_i^α self-consistently.

Thus the system within the present model may be described with the following phenomenological parameters: the energy E_0 , the Coulomb integral U , the hopping integral V , which we assume to be nonzero only for nearest neighbors, and the level width Γ . Usually it is more convenient to use dimensionless variables $x_i = (E_{0i} - \epsilon_F)/\Gamma$, $y_i = U_i/\Gamma$, and V/Γ . In this case all the energies are expressed in units of Γ .

We assume that the magnitudes of the parameters x_i , y_i , and V/Γ have been determined from calculations of properties of the homogeneous sample and V/Γ is taken to be the same for both the materials. Were more comprehensive information available regarding the parameters involved, these restrictions could be easily lifted.

In the present study we have investigated the nature of the magnetic order in the surface alloy of Fe and Cr atoms. This implies attributing to each site the values of the parameters E_{0i} and U_i and the initial spin occupation numbers for the corresponding type of atom in the bulk. While this initial step is performed one has to solve the set of Eqs. (11), (13), and (17), calculating the diagonal matrix elements of the self-energy matrix σ_i^α for each i and spin polarization α :

$$\sigma_i^\alpha = \sum_{j \in \mathcal{M}_i^{(l)}} \frac{V^2}{\omega - E_j^\alpha} \quad (18)$$

(This formula is obtained for the bcc lattice that corresponds to the system under consideration; the summation proceeds over all the sites inside the first coordination sphere of the i th site.) With this expression for σ_i^α one may represent the diagonal Green functions as a sum of simple pole terms. Although this involves solving ninth-degree equations at each site, the algorithm for this is fairly fast. Since the integrals of Eq. (17) can be evaluated analytically, this method of calculation seems to be most ergonomic. After the integrals have been calculated, the set of the self-consistent equations (13) can be written implicitly at each site for both the spin polarizations. Thus the procedure results in a set of equations for the unknown spin occupation numbers at each site.

The system obtained is overly complicated for an explicit presentation, but fortunately one may deal with it quite effectively with a straightforward iterative treatment; namely, the initial values of the spin occupation numbers are taken to be equal to the corresponding values for the bulk material. These numbers can then be recalculated with the system described above and taken as the occupation numbers for the next step, and so forth until the spin occupation numbers cease to change.

The procedure is quite stable, although it is impossible to guarantee the uniqueness of the solution obtained. One has to calculate the magnitude of the energy (or free energy for the finite-temperature case) for each configuration obtained and choose the lowest-energy configuration. (It has to be noted that the corresponding

energies deviate only slightly and consequently a few solutions may appear physically meaningful as metastable states.) We postpone discussion of this problem for a forthcoming publication. However, it is obvious that such an investigation requires much more powerful computer facilities than we presently have at our disposal.

One more procedure in our program fits the Fermi energy, which fixes the total number of electrons in correspondence with the density of the added Cr atoms. The fitting procedure is straightforward and requires repetition of the algorithm described above a few times with different values of the Fermi energy. This procedure is also quite stable, but it increases the run time significantly. Of course, fitting of the Fermi energy is reasonable only if the number of Fe layers is quite small; otherwise the value of the Fermi energy is fixed to be equal to its value in the bulk.

This brief description of the present scheme exhausts the strategy of the calculations. Some preliminary studies were performed for tuning the routine; namely, a series of calculations was accomplished for some special configurations of the Fe-Cr atoms on the surface, which had been studied previously^{13,16} by a quite different method. These results deserve a separate discussion elsewhere; here we only state that for all the configurations considered a reasonable correspondence between the results of the different approaches was obtained.

IV. RESULTS OF CALCULATIONS

It was reported previously¹⁴ that a Cr atom, being embedded in an Fe environment, can significantly change the local magnetic ordering, substantially damping the magnetic moments of the surrounding Fe atoms. Consequently, Cr atoms placed deeply into a Cr/Fe interface may cause a significant decrease of the interface magnetic moment, as has been observed in Ref. 10.

To scrutinize this hypothesis, we have constructed two different ensembles representing the Fe-Cr interface. In the first case all the atoms are sputtered on the initially filled layer of Fe with the A variant of the EPITAXY algorithm. The interfaces obtained are not regular, but do not contain any empty sites inside the interface.

In the second series the interfaces are much more rumpled. First, 6×64 Fe atoms are nested onto the initial, completely filled, Fe layer with the B variant of the EPITAXY algorithm. This procedure results in quite "shaggy" patterns which usually contain sharp apices, gorges, hollows, and even caves. After the Fe part of the interface is formed, the number of Cr atoms fixed by the coverage parameter ζ is thrown upon the top of the prism, while their descent is treated within the A variant of the EPITAXY algorithm.

Analyzing the Figs. 2(a), one may infer that the structures of the Fe surfaces, obtained within the B algorithm, are porous and only the lowest 18th level, which is completely filled *ad hoc*, terminates the invasion of the empty states into the Fe bulk. This makes the present variant of the epitaxy modeling less realistic, but it hardly spoils the results obtained. This variant of the procedure allows also Cr atoms to penetrate deep into the shaggy Fe pat-

tern, in qualitative correspondence with exponential law. As a result, the cavities in the Fe surface appear to be partly filled with Cr atoms (especially the cavities which are close to the interface) and the interface becomes smoother. This provides the condition for the mechanism exposed above to be operative.

Definitely, our method of epitaxial interface modeling is not unique. However, we do suggest that it is the most natural algorithm giving rise to strongly intermixed surface alloys and its elevation for detailed modeling of such alloys requires much more detailed information on the epitaxial growth mechanism.

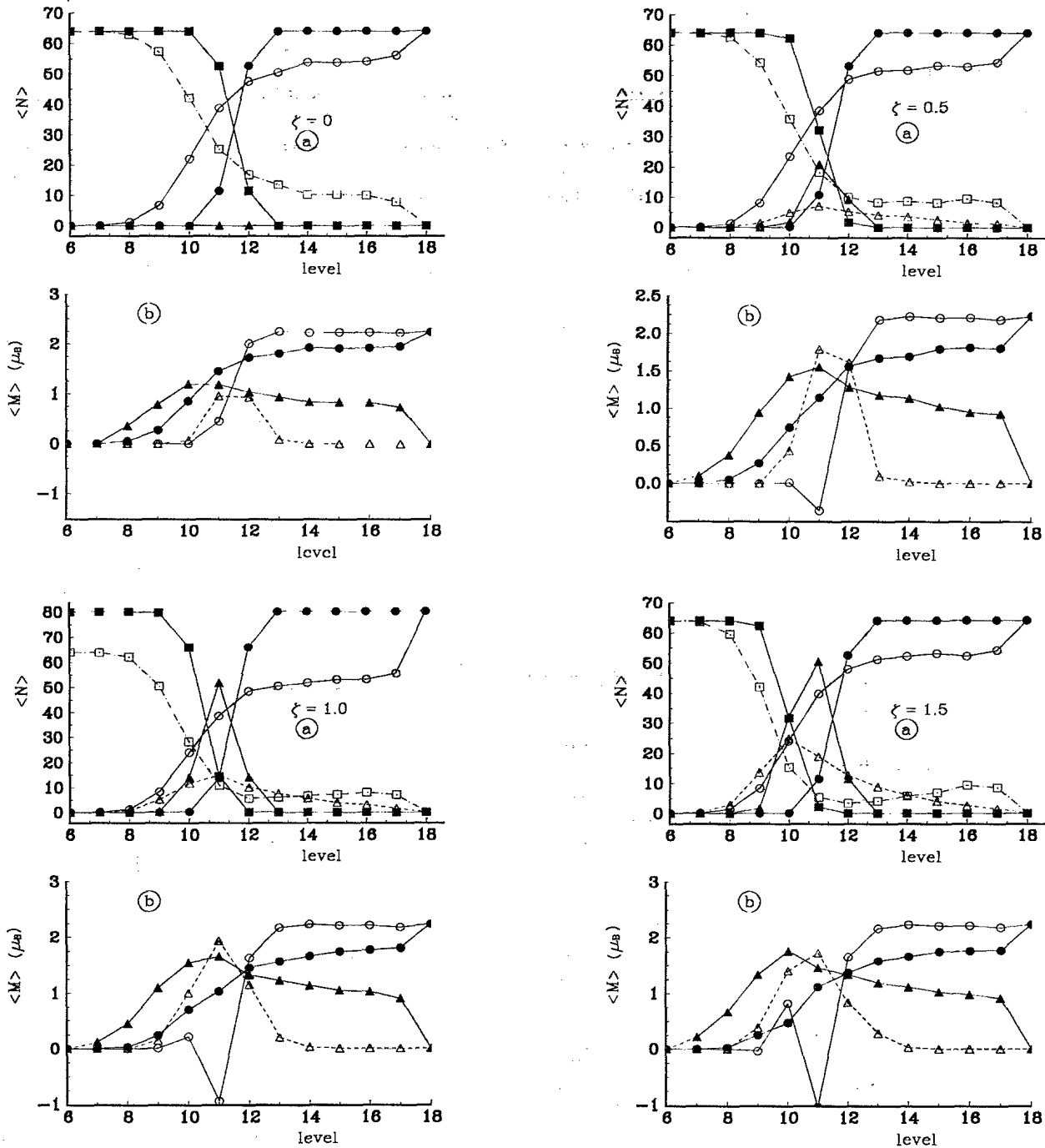


FIG. 2. This set of figures expose the principal results of our calculations. The dependences of the averaged amounts of atoms $\langle N \rangle$ of different types (a) and the averaged magnetic moment of the layers (b) in dependence on the number of layers are presented for different values of the coverage number ζ . In (a) the circles and solid lines correspond to the Fe atoms, the triangles linked with the dotted lines stand for the Cr atoms, and the boxes linked with the dash-dotted lines represent the empty sites. In (b) the solid circles linked with the solid lines represent the magnetic moments and the triangles linked with the dotted lines give the dispersion $\delta = (\langle m^2 \rangle - \langle m \rangle^2)^{1/2}$ of the magnetic moments. The empty symbols depict the results obtained within the A variant of the EPITAXY algorithm while the solid symbols give the results within the mixed variant of this algorithm.

Let us consider the results obtained. In Fig. 3 the magnetic moment of the layer (per one atom) in dependence on the number of the level is represented for a few different values of the coverage parameter ζ . These curves correspond to the simplest uniform coverage of the interface and therefore such a construction is available only for integer values of the parameter ζ . They clearly demonstrate the essential features of this ideal system.

(i) If the Fe surface is not covered by Cr, the magnetic moments of the surface Fe atoms are slightly greater than

they are in the bulk. This phenomenon was discussed previously within the present model¹⁴ and within the density-functional approach.²² The moment increase obtained within the present framework is smaller than that given in Ref. 22, although, if the parameters of the Fe d subsystem in the bulk are slightly changed, we can reproduce the results obtained with the density-functional method. By the way, a slight change of the parameters of the model (the first suspect is the hopping parameter V) for the surface atoms may be caused by some reconstruction of the surface.

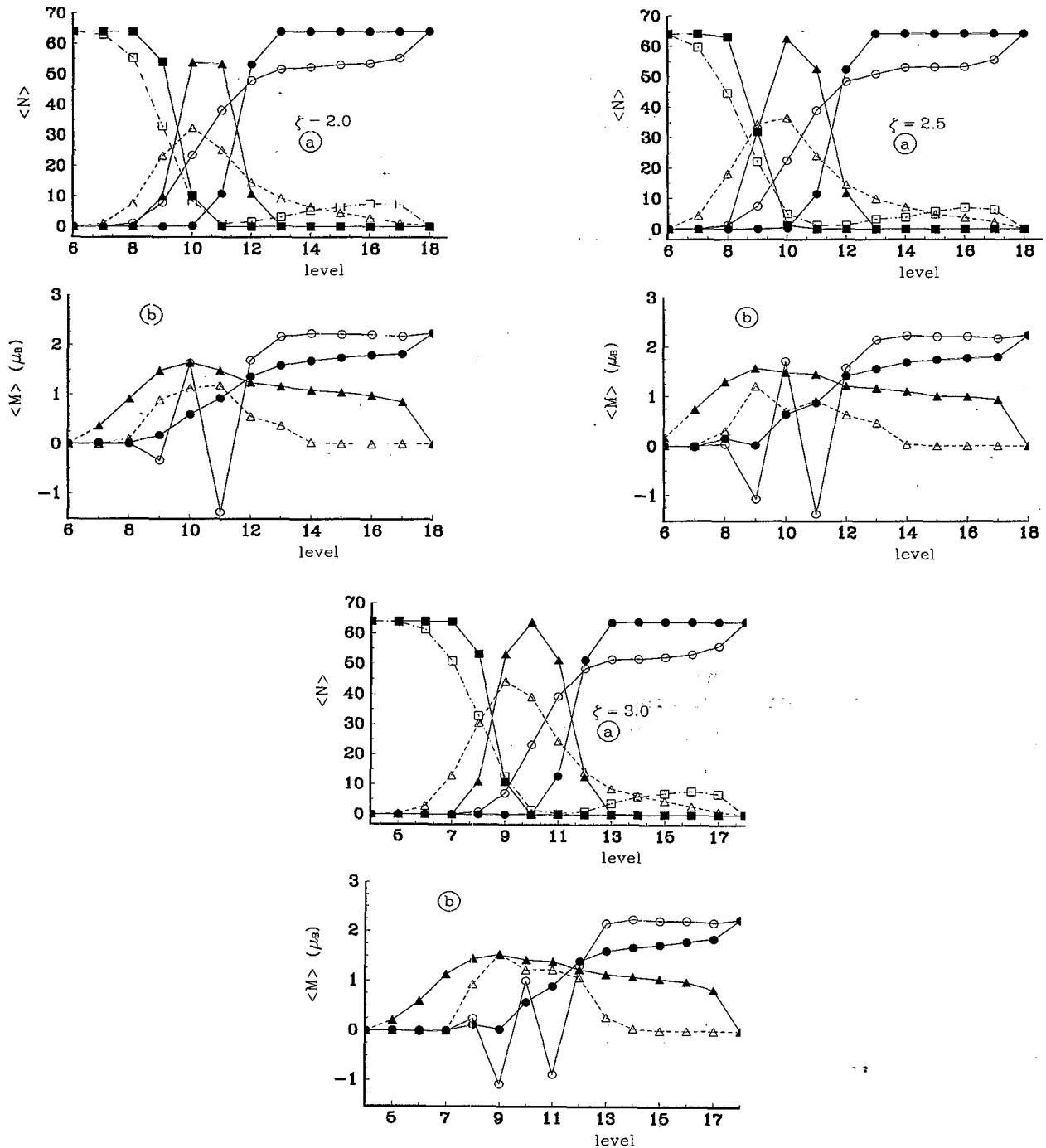


FIG. 2. (Continued).

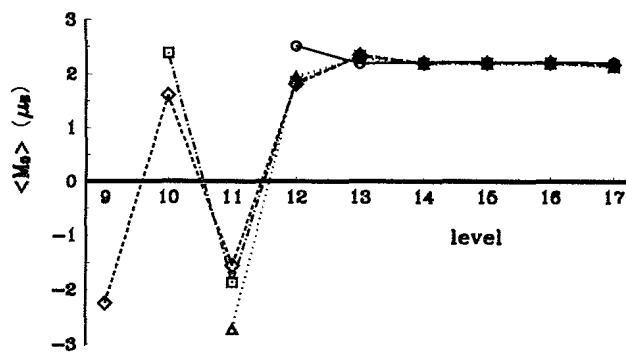


FIG. 3. The magnetic moments per one site in the layer in dependence on the level number are depicted for the case of the regular structure of the interface. The circles correspond with the vicinal Fe surface; the triangles show the result for the Cr monolayer coverage onto this Fe surface; squares and diamonds depict the results for two and three monolayers of Cr on the Fe surface.

(ii) The first layer of Cr atoms is ordered antiferromagnetically with respect to the Fe bulk. This result seems to be universally obtained theoretically,^{13,14} and experimentally.^{10,6}

(iii) The Cr coverage reveals antiferromagnetic ordering. With the coverage parameter ζ increase, the magnitude of oscillation sweeps decreases inward in the newly formed Cr "bulk."

The dependences of the average magnetic moments on the interface level number for randomly created interfaces are depicted in Figs. 2(b). The most impressive result in these figures is the drastic difference between the two interfaces considered. The first algorithm provides a more regular interface, in which there are no holes and the Fe-Cr intermixing is localized in well-defined regions. In this case the average magnetic ordering resembles pretty much (even quantitatively) the pictures (Fig. 3) obtained for the most regular, homogeneous structures. In both cases the prominent antiferromagnetic ordering in the Cr coverage and the antiferromagnetic orientation of the first Cr layer with respect to the Fe bulk are clearly exposed.

Nothing of this can be seen in Figs. 2(b) for the mixed A and B algorithm. In the case of "shaggy" epitaxial interfaces the magnetic ordering of the interface is ferromagnetic on average. One may say that the Fe ferromagnetic order frustrates the freedom of the Cr magnetic moments. This is due to strong absorption of the Cr atoms by the rather porous Fe interface, which works as a blotting paper. Only a few Cr atoms appear to be free of the influence of the Fe environment and they fail to organize themselves, segregating their community from the ferromagnetic bulk. Of course, this occurs because our random procedure leads to an extremely porous construction of the Fe subsystem, in which the concentration of empty sites does not decrease inward in the Fe bulk.

Actually, one may assume that the holes in the Fe bulk would be saturated by some amount of Cr atoms and

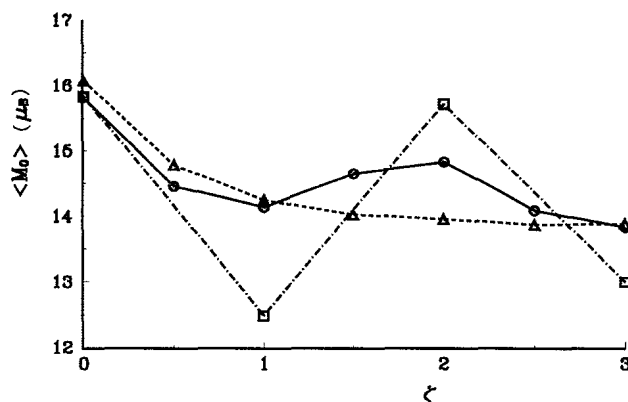


FIG. 4. The magnetic moments of the sample per one surface cell in dependence on the coverage parameter ζ are plotted for both the series considered. The circles and solid line correspond to the more regular (A) interfaces, while triangles and the dotted line represent the result of calculations for the "shaggy" interface. For comparison, with the squares and the dash-dotted line we give the results of the calculations for regular coverage.

then these atoms commence nesting onto the surface of the already smooth Fe/Cr interface. As a result, for small values of the coverage parameter ζ the magnetic order of the interface follows the behavior presented in Fig. 3, while after the holes in the Fe bulk are saturated one may assume the transformation of the magnetic ordering pattern toward the antiferromagnetic ordering of the Cr cover.

It is instructive to follow the dependence of the mean square deviation of the magnetic moment $\delta = \langle (m^2 - \langle m \rangle^2)^{1/2} \rangle$ in the different levels on the type of EPITAXY algorithm. However, one should not overestimate the physical meaning of this quantity, since it is overly average to represent the degree of randomness of the magnetic ordering in the interface. Actually, this randomness can be described with the correlation functions of the moments in the different layers, etc. Nevertheless, the quantity δ clearly demonstrates to what extent the randomness can influence the magnetic ordering and demonstrates the regions in which the disorder influence substantially reveals itself. However, we suggest that the total magnetic moment of the sample is the only physical quantity which can be measured reasonably. We are quite pessimistic regarding the possibility of accurate experimental probing of the average magnetic-moment dependence on the level number.

The magnetic moments of the sample in dependence on the coverage parameter ζ are plotted on Fig. 4 for both the series considered. The circles and solid line correspond to the more regular (A) interfaces, while triangles and the dotted line represent the result of calculations for the "shaggy" interface. For comparison, with the squares and the dash-dotted line we give the results of the calculations for the regular coverage. The results for these "shaggy" interface are in qualitative agreement with experiment.¹⁰

V. RÉSUMÉ

The EPITAXY routine which allows one to simulate the properties of the Fe-Cr interfaces is developed. The algorithm works in two variants. One of them provides more regular structures while the second algorithm generates quite irregular interfaces. For sets of the interfaces, constructed with the EPITAXY algorithm for different values of the coverage parameter ξ and consisting of 30 configurations, self-consistent calculations of the magnetic properties of the systems are performed. This allows us to obtain the average physical quantities of the interface in dependence on ξ with reasonable accuracy.

It is shown that partial coverage of the Fe vicinal surface by chromium causes a decrease in the average magnetic moment of the interface. This is due to penetration of the Cr atoms into the interface, which results in a decrease of the magnetic moments of the neighboring Fe atoms. In addition Cr atoms couple antiferromagnetically to the neighboring Fe atoms. A substantial role of the surface roughness in smoothing out the coverage-dependent average magnetic-moment oscillations is revealed.

The present method of study of the magnetic properties of rough interfaces seems to be a quite useful investigation tool due to its universality and the relative simplicity of the calculations. For simpler systems the method

gives results in good agreement with other well-established schemes such as the Hubbard model²³ and the density-functional method.²² However, our approach makes it possible to describe much more complex systems, which cannot be investigated within the traditional Hubbard model and within *ab initio* theories. We restrict ourselves to accounting for the *d-d* interaction only inside the nearest-neighboring sphere, although, as was evidenced by our previous calculations,²¹ this does not substantially influence the results obtained.

We would like to note that our results are in good qualitative agreement with the available experimental data, bearing in mind that the different experimental methods of investigation give rather deviating results. This is very natural, since the systems under investigation, as well as the methods of their experimental study, are rather subtle. Therefore one has to wait until the final judgment on the correspondence between the present theory and experiment may be formulated in more definite terms.

ACKNOWLEDGMENTS

V.M.U. is thankful for financial support of this work by the Russian Fund of Fundamental Investigations (Grant No. 93-03-5644) and the International Scientific Fund (Grant No. R62000)

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- ¹M. N. Babich, J. M. Broto, A. Fert, F. Nguyen van Dau, F. Petroff, P. Etienne, G. Creuzet, A. Friedrich, and J. Chazelas, *Phys. Rev. Lett.* **61**, 2472 (1988).
- ²S. S. P. Parkin, N. More, and K. P. Roche, *Phys. Rev. Lett.* **64**, 2304 (1990).
- ³P. Grünberg, R. Schreiber, P. Yang, M. B. Brodsky, and H. Sowers, *Phys. Rev. Lett.* **57**, 2442 (1986).
- ⁴S. S. P. Parkin, *Phys. Rev. Lett.* **67**, 3598 (1991).
- ⁵J. Unguris, R. J. Celotta, and D. T. Pierce, *Phys. Rev. Lett.* **67**, 140 (1991).
- ⁶J. Unguris, R. J. Celotta, and D. T. Pierce, *Phys. Rev. Lett.* **69**, 1125 (1992); D. T. Pierce, R. J. Celotta, and J. Unguris, *J. Appl. Phys.* **73**, 6201 (1993).
- ⁷Y. U. Idzerda, L. H. Tjeng, H.-J. Lin, G. J. Gutierrez, G. Meigs, and C. T. Chen, *Phys. Rev. B* **48**, 4144 (1993); *J. Appl. Phys.* **73**, 6204 (1993).
- ⁸F. U. Hillebrecht, Ch. Roth, R. Jungblut, E. Kisker, and A. Bringer, *Europhys. Lett.* **19**, 711 (1992).
- ⁹T. G. Walker, A. W. Pang, H. Hopster, and S. F. Alvarado, *Phys. Rev. Lett.* **69**, 1121 (1992).
- ¹⁰C. Turtur and G. Bayreuther, *Phys. Rev. Lett.* **72**, 1557 (1994).
- ¹¹J. Xu and A. J. Freeman, *Phys. Rev. B* **47**, 165 (1993).
- ¹²M. Schilfgaarde, and F. Herman, *Phys. Rev. Lett.* **71**, 1923 (1993).
- ¹³A. Vega, L. C. Balbás, A. Chouairi, H. Dreyssé, and C. Demangeat, *Phys. Rev. B* **49**, 12 797 (1994).
- ¹⁴V. N. Gittsovich, V. G. Semenov, and V. M. Uzdin, *J. Magn. Magn. Mater.* **146**, 165 (1995).
- ¹⁵A. K. Kazansky, A. S. Kondrat'ev, and V. M. Uzdin, *Fiz. Met. Metalloved.* **71**, 53 (1990).
- ¹⁶A. Vega, C. Demangeat, H. Dreyssé, and A. Chouairi, *Phys. Rev. B* **51**, 11 546 (1995).
- ¹⁷A. K. Kazansky and V. M. Uzdin, *Fiz. Met. Metalloved.* **76**, 53 (1993).
- ¹⁸A. K. Kazansky, A. S. Kondrat'ev and V. M. Uzdin, *Sov. Phys. JETP* **67**, 372 (1988).
- ¹⁹Y. Teraoka and J. Kanamori, *Physica B+C* **91B**, 199 (1977).
- ²⁰Y. Teraoka, *Prog. Theor. Phys. Suppl.* (101), 181 (1990).
- ²¹A. K. Kazansky and V. M. Uzdin, *Fiz. Tverd. Tela (Leningrad)* **32**, 3384 (1990) [*Sov. Phys. Solid State* **32**, 1958 (1990)].
- ²²A. J. Freeman, *J. Magn. Magn. Mater.* **100**, 497 (1991).
- ²³C. Demangeat and V. M. Uzdin (unpublished).