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Magnetic structure of FCC iron

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Abstract. A generalization of the LMTO method for the case of crystals with spiral magnetic structure is suggested. The method is used for self-consistent calculations of electronic and magnetic properties of spiral magnetic configurations of FCC iron. The atomic volumes considered cover the region of known low-spin to high-spin transitions in ferromagnetic FCC iron. The dependence of electronic properties on the spiral vector and number of valence electrons is investigated. The total energy minimum corresponds to a non-collinear magnetic structure, in accordance with recent experimental data.

1. Introduction

The magnetic and electronic properties of FCC iron (γ -Fe) have been traditionally the subject of many investigations (see, e.g., experimental [1–4] and theoretical papers [5–8]). These are concerned with both the fundamental significance of γ -Fe properties for the understanding of the physical nature of 3d metallic magnetism and also the practical interest in FCC iron alloys which show the Invar anomaly. An explanation of this anomaly is based on the peculiarities of magnetic properties of FCC Fe [9].

On the other hand, information about the magnetic structure and electronic properties of γ -Fe remains contradictory owing mainly to difficulties with the experimental investigation of FCC iron at low temperatures. In most of the investigations, the presence of two stable magnetic states of FCC Fe has been pointed out: low spin (LS) and high spin (HS). However, contrary points of view have been expressed on the types of magnetic structure corresponding to these states. So, it follows from the results of [5–8] that the LS state has an antiferromagnetic (AFM) structure, but the HS state has a ferromagnetic (FM) structure. In [10], the opposite conclusion was drawn. Finally, in more recent measurements [4] for γ -Fe alloy precipitates with a small amount of Co it was pointed out that FCC Fe precipitates have a spiral-spin-density-wave (SSDW) structure. This result is consistent with theoretical estimations [11] obtained on the basis of calculations of the unenhanced magnetic susceptibility of FCC Fe.

The purpose of the present paper is to present the first direct band-structure calculations of the electronic and magnetic properties of γ -Fe with different SSDWs cor-

responding to the spiral vector $\mathbf{q} = (0, 0, q)$. In particular for $q = 0$ and $q = 1$ (in $2\pi/a$ units, where a is the lattice constant) we obtain FM and AFM structures correspondingly.

A direct calculation of the electronic properties of spiral magnetic configurations has become possible after a variety of methods of non-collinear magnet band-structure calculations have been proposed [12–14]. In [12, 13] it was shown that, by taking into account a generalized symmetry of the Hamiltonian of a spiral magnet, it is possible to simplify the calculations considerably. In [13], generalizations of the Korringa–Kohn–Rostoker (KKR) method, the augmented plane-wave method and the tight-binding method have been carried out for the case of crystals with a spiral magnetic structure. The present work is based on the formalism of the linearized muffin-tin orbital (LMTO) method [15].

The paper is organized as follows. In section 2 the derivation of the secular equation and Hamiltonian of the LMTO method for crystals with a spiral magnetic structure is given (we shall use the abbreviation LMTO-ss for this method). The peculiarities of the one-electron potential construction are discussed. In section 3 we present the results of the calculations carried out for spiral configurations of FCC iron. Various values of the Wigner–Seitz radius are considered. A discussion of the main results is given.

2. Method of calculation

Let us consider a crystal with a SSDW defined in the atomic sphere approximation by the following spin-density distribution $\mathbf{m}(\mathbf{r})$:

$$\mathbf{m}(\mathbf{r}) = \sum_i \eta(|\mathbf{r} - \mathbf{r}_i|) |\mathbf{m}(|\mathbf{r} - \mathbf{r}_i|)| \mathbf{e}_i \quad (1a)$$

$$\mathbf{e}_i = \{\sin(\theta) \cos(\mathbf{q} \cdot \mathbf{r}_i), \sin(\theta) \sin(\mathbf{q} \cdot \mathbf{r}_i), \cos(\theta)\} \quad (1b)$$

where \mathbf{r}_i is the radius vector of the i th atom, $\eta(|\mathbf{r} - \mathbf{r}_i|)$ is the function equal to unity within the atomic sphere i and to zero outside it, θ is the angle between atomic moments and the global z axis, \mathbf{e}_i is a unit vector determining the direction of the magnetic moment of atom i , and \mathbf{q} is the spin-spiral vector defining the angle between the magnetic moments of neighbouring layers.

Non-collinearity of magnetic moments leads to the loss of translational symmetry of the crystal. This makes it difficult to investigate the electronic structure of non-collinear magnets. If the period of the magnetic structure is commensurate with the period of lattice, considerations may be restricted to the magnetic unit cell. However, in this case the amount of calculations increases sharply. For incommensurate structures the traditional approach is in principle inapplicable. On the other hand, in [12, 13] it was shown that the one-electron Hamiltonian of the spiral magnet possesses a generalized symmetry, which can restrict consideration to the chemical unit cell. In this case the calculations of the electronic structure become not much more complicated than in case of FM ordering. Below we discuss a formalism for the LMTO calculations of the energy bands of crystals with a SSDW structure.

2.1. LMTO method for crystals with a spiral magnetic structure

Here we give the derivation of the LMTO-ss method focused on the difference between secular matrices of a ferromagnet and those of crystals with a SSDW structure.

In a site representation the secular equation of the LMTO method for a crystal with FM ordering has the form

$$\det \|\mathbf{g}^{-1}\| = 0 \quad (2)$$

where the matrix \mathbf{g}^{-1} is expressed through the potential function $\mathbf{P}(E)$ of the LMTO method, and the structure constant S :

$$\bar{g}_{iL\alpha, jL'\beta}^{-1} = (P_{iL\alpha}(E)\delta_{ij}\delta_{LL'} - S_{iL\alpha, jL'\beta})\delta_{\alpha\beta}. \quad (3)$$

The matrix \mathbf{P} characterizes the scattering properties of an individual atom and is diagonal with respect to the site indices, i and j , the orbital indices $L = (l, m)$ and $L' = (l', m')$, and the spin indices α and β . In the case of a ferromagnet a global axis of spin quantization is chosen to be parallel to the direction of atomic moments. The potential function may be easily found if the one-electron potential within the atomic sphere is known. For the potential function it is convenient to use the formula [15]

$$P_{iL\alpha}(E) = \Gamma_{iL\alpha}/(\mathbf{V}_{iL\alpha} - E) + \mathbf{Q}_{iL\alpha} \quad (4)$$

where Γ , \mathbf{V} and \mathbf{Q} are the potential parameters of the LMTO method.

In the case of a spiral magnetic structure (1) the $\mathbf{P}(E)$ -matrix is not diagonal in spin indices. However, the $\mathbf{P}(E)$ -matrix block corresponding to the i th atom is diagonal in the local coordinate system where the spin quantization axis is parallel to the atomic moment of the i th atom. This property is a consequence of the corresponding property of the reversed single-site \mathbf{t} -matrix from which $\mathbf{P}(E)$ can be obtained after a number of simplifications [15]. Transformation of the i th block of $\mathbf{P}(E)$ -matrix from the local coordinate system associated with the i th atom into the global coordinate system can be carried out by using a spin- $\frac{1}{2}$ rotation matrix \mathbf{U}_i . In particular for a spin density distribution (1) we use a $\mathbf{U}_i(\theta, \mathbf{q})$ matrix:

$$\mathbf{U}_i(\theta, \mathbf{q}) = \begin{pmatrix} \cos(\theta/2) \exp(i/2\mathbf{q} \cdot \mathbf{r}_i) & \sin(\theta/2) \exp(-i/2\mathbf{q} \cdot \mathbf{r}_i) \\ -\sin(\theta/2) \exp(i/2\mathbf{q} \cdot \mathbf{r}_i) & \cos(\theta/2) \exp(-i/2\mathbf{q} \cdot \mathbf{r}_i) \end{pmatrix}. \quad (5)$$

For fixed i, L, α this transformation is defined by the formula

$$\bar{P}_{iL\alpha, \beta} = \sum_{\beta'} U_{i\alpha\beta'}(\theta, \mathbf{q}) P_{iL\beta'} U(\theta, \mathbf{q})_{\beta\beta'}^{-1}. \quad (6)$$

As the structure constant matrix \mathbf{S} depends only on the crystal lattice, the secular equation of a non-collinear magnet may be written as follows:

$$\det \|\mathbf{U}\mathbf{P}\mathbf{U}^{-1} - \mathbf{S}\| = 0. \quad (7)$$

Here, a \mathbf{P} -matrix block for any atom i is written in its own local coordinate system, and the \mathbf{U} -matrix is composed of individual \mathbf{U}_i -matrices. It is useful to rewrite (7) as follows:

$$\det \|\bar{\mathbf{g}}^{-1}\| = \det \|\mathbf{P} - \tilde{\mathbf{S}}\| = 0 \quad (8)$$

where

$$\bar{g}_{L\alpha, L'\beta}^{-1} = P_{iL\alpha}(E)\delta_{ij}\delta_{LL'}\delta_{\alpha\beta} - \sum_{\alpha', \beta'} U_{i\alpha\alpha'}^{-1} S_{iL\alpha', jL'\beta'} U'_{j\beta'\beta}. \quad (9)$$

Replacing the basis functions corresponding to the form (9) of the secular matrix by their Bloch sums, we obtain a unitary transformation of the secular matrix:

$$\bar{g}_{L\alpha, L'\beta}^{-1}(\mathbf{k}, \mathbf{k}') = \frac{1}{N} \sum_{i \neq j} \exp(-i\mathbf{k}' \cdot \mathbf{r}_i) \bar{g}_{iL\alpha, jL'\beta}^{-1} \exp(+i\mathbf{k}' \cdot \mathbf{r}_j) \quad (10)$$

where N is the number of atoms. Taking into consideration the actual form of the matrices $\mathbf{U}_i(\theta, \mathbf{q})$ for the spiral magnetic structure (1), we obtain the following expression for the matrix (10):

$$\tilde{g}_{L\alpha L'\beta}^{-1}(\mathbf{k}, \mathbf{k}') = [P_{L\alpha}(E)\delta_{LL'}\delta_{\alpha\beta} - \tilde{S}_{L\alpha L'\beta}]\delta(\mathbf{k} - \mathbf{k}'). \quad (11)$$

Here the matrix $\tilde{\mathbf{S}}$ is defined by the formula

$$\begin{aligned} \tilde{S}_{L\alpha L'\beta}(\mathbf{k}) = S_{LL'}(\mathbf{k} - \mathbf{q}/2) & \begin{pmatrix} \cos^2(\theta/2) & -\frac{1}{2}\sin(\theta) \\ -\frac{1}{2}\sin(\theta) & \sin^2(\theta/2) \end{pmatrix} \\ + S_{LL'}(\mathbf{k} + \mathbf{q}/2) & \begin{pmatrix} \sin^2(\theta/2) & +\frac{1}{2}\sin(\theta) \\ +\frac{1}{2}\sin(\theta) & \cos^2(\theta/2) \end{pmatrix} \end{aligned} \quad (12)$$

where $S_{LL'}(\mathbf{k})$ are the structure constants of the traditional LMTO method [15]. The diagonality of the matrix (11) with respect to the wavevector index is a non-trivial result in the case of a non-collinear structure. It is a consequence of the generalized symmetry of the problem that was discussed in [12]. The form (11) of the secular matrix of the LMTO-SS method is very close to the corresponding formula for the KKR-SS method [13].

The secular equation (8) can be rewritten in the form

$$\det \|\mathbf{E} - \tilde{\mathbf{H}}\| = 0 \quad (13)$$

where the Hamiltonian $\tilde{\mathbf{H}}$ of the LMTO-SS method is defined by formula

$$\tilde{H}_{L\alpha L'\beta}(\mathbf{k}) = V_{L\alpha}\delta_{LL'}\delta_{\alpha\beta} + \Gamma_{L\alpha}^{1/2}[Q - \tilde{S}(\mathbf{k})]_{L\alpha L'\beta}^{-1}\Gamma_{L'\beta}^{1/2}. \quad (14)$$

In (14), Γ , V and Q are the potential parameters defined by equation (4). So, the secular equation of the problem is constructed from the same quantities as the secular equation of the traditional LMTO method. However, in contrast with the traditional method, the Hamiltonian (14) is non-diagonal in the spin indices. It is a result of the hybridization of electronic states with opposite spin projections.

A substantial simplification of the calculations follows from the symmetry properties of the electronic energy spectrum in reciprocal space. In the case of a spiral structure these properties have some important peculiarities as discussed in [12, 13]. In the present paper we deal with spiral magnetic configurations of FCC Fe which are characterized by the vector \mathbf{q} parallel to the z axis and deviating from it by an angle $\theta = 90^\circ$. For these structures, the spectrum symmetry may be described by the traditional formula

$$\varepsilon(\alpha_R \mathbf{k}) = \varepsilon(\mathbf{k}) \quad (15)$$

where α_R are rotational operations of the cubic group satisfying one of the following equalities:

$$\alpha_R \mathbf{q} = \mathbf{q} \quad (16a)$$

$$\alpha_R \mathbf{q} = -\mathbf{q}. \quad (16b)$$

As a result, calculations were carried out for vectors \mathbf{k} belonging to one eighth of the Brillouin zone of the FCC lattice.

2.2. The construction of the potential

In order to find the self-consistent potential of a non-collinear magnet we followed the general density functional scheme described in [16, 17]. The total energy of a crystal may be represented in the form of a functional

$$E[n, m] = T + E_H[n] + E_{xc}[n, m] \quad (17)$$

$$m(\mathbf{r}) = \sum_i \psi_i^\dagger(\mathbf{r}) \boldsymbol{\sigma} \psi_i(\mathbf{r}) \quad n(\mathbf{r}) = \sum_i \psi_i^\dagger(\mathbf{r}) \psi_i(\mathbf{r}) \quad (18)$$

where T is the kinetic energy, E_H and E_{xc} are the Hartree and exchange–correlation contributions, respectively and $\boldsymbol{\sigma}$ are the Pauli matrices. Variation in the functional (17) with respect to $n(\mathbf{r})$ and $m(\mathbf{r})$ leads to the one-electron Kohn–Sham equations

$$(-\nabla^2 \delta_{\alpha\beta} + V_{\alpha\beta}^{\text{eff}}) \psi_{\beta i}(\mathbf{r}) = \varepsilon_i \psi_{\alpha i}(\mathbf{r}). \quad (19)$$

The effective potential V^{eff} includes the Hartree exchange–correlations contributions:

$$V_{\alpha\beta}^{\text{eff}} = V_{\alpha\beta}^H + V_{\alpha\beta}^{\text{xc}} \quad (20)$$

$$V_{\alpha\beta}^H + 2\delta_{\alpha\beta} \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 r' \quad V_{\alpha\beta}^{\text{xc}} = V[n, m] + \mathbf{B}[m] \boldsymbol{\sigma} \quad (21)$$

$$V[n, m] = \frac{1}{2} \partial E_{xc}(n, m) / \partial n \quad \mathbf{B}[n, m] = \frac{1}{2} \partial E_{xc}(n, m) / \partial m. \quad (22)$$

The ground state of a system of interacting electrons may be described by equations (18)–(22) being solved self-consistently.

The SSDW is one of the possible excitations of a system of interacting electrons. In this case it is necessary to consider the extension of density functional theory to a constrained system [18, 19]. The total energy functional for crystals with fixed magnetic moment orientations is modified as follows:

$$E^*[n, m] = E[n, m] + \sum_i \int_{v_i} d\mathbf{r} \{ \mathbf{h}(\mathbf{r}) \cdot [m(\mathbf{r}) - \mathbf{e}_i |m(\mathbf{r})|] \} \quad (23)$$

where $\mathbf{h}(\mathbf{r})$ is the Lagrange parameter which has the meaning of a field responsible for the fulfilment of the constraining condition imposed by equation (1). In (23), v_i is the volume of the i th atomic sphere. Since all atoms are equivalent in the local coordinate system, we can restrict ourselves to the consideration of one atomic sphere only, with $\mathbf{e}_i = \mathbf{e} = (0, 0, 1)$. Variation in (23) leads to a modified potential within one atomic sphere, in the local coordinate system associated with the i th atom:

$$\mathbf{B}^*[n, m] = \mathbf{B}[n, m] + \mathbf{h}[\mathbf{r}, m] - (\mathbf{h}[\mathbf{r}, m] \cdot \mathbf{e}) m(\mathbf{r}) / |m(\mathbf{r})|. \quad (24)$$

However, taking into consideration the condition fixing the moment orientation, i.e.

$$m(\mathbf{r}) - e|m(\mathbf{r})| = 0 \quad (25)$$

we have, in the local-density-functional approximation $E_{xc}[n, m] \approx \tilde{E}_{xc}[n, |m|]$,

$$\mathbf{B}^*[n, |m|] = \frac{1}{2} [\partial \tilde{E}_{xc}(n, |m|) / \partial |m(\mathbf{r})|] \mathbf{e}. \quad (26)$$

For $\tilde{E}_{xc}[n, |m|]$ we used the von Barth–Hedin [16] formula. To sum up, on each step of the iterational process, the potential V^{eff} defined by equations (20)–(22) and (26) is used to find the potential parameters corresponding to the axis of spin quantization. These parameters are used further to solve the secular equation (13). The electronic eigen-

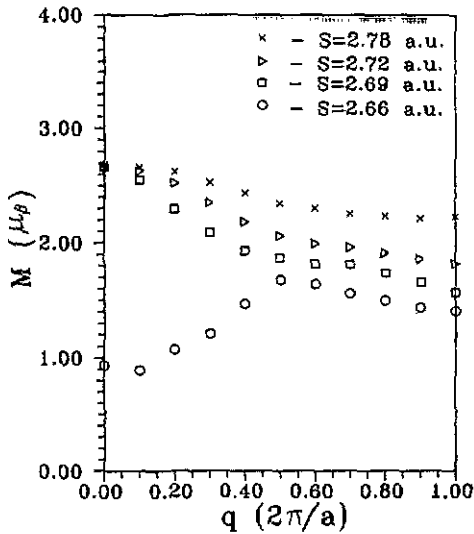


Figure 1. Local magnetic moment of FCC Fe as a function of the spiral vector magnitude.

functions thus obtained correspond to the local coordinate system and enable the projection of magnetic density within an atomic sphere in the ϵ direction to be found easily. Using (20)–(22) and (26) we immediately obtain the potential for the next step of the iterational process.

3. Results

The magnetic and electronic properties of FCC Fe have been discussed intensively [5–8], but only collinear magnetic configurations have been taken into account thus far. We applied the above-described method for the investigation of SSDWs in FCC Fe. The spin spiral magnetic configurations with vector $\mathbf{q} = q(0, 0, 1)$ and $\theta = \pi/2$ were considered. In particular for $q = 0$ and $q = 1$ we considered FM and AFM structures correspondingly.

The results of self-consistent LMTO-SS calculations of the local magnetic moment $m(q)$ as a function of absolute value q of the spin-spiral vector for FCC Fe at different Wigner-Seitz radii (S) are shown in figure 1. For spiral configurations close to the FM structure ($q = 0$) the results of our calculations are very sensitive to the lattice constant. The value of the magnetic moment changes from $M = 1.0 \mu_B$ at $S = 2.66$ au to $M = 2.7 \mu_B$ at $S = 2.78$ au. Thus, in this range of lattice constants the transition from the LS state at a smaller volume ($S = 2.66$ au) to the HS state at a larger volume ($S = 2.69$ au) takes place. These results are in accordance with those of [6], obtained by the full-potential linearized-augmented-plane-wave method and fixed-spin-moment method [7, 8] for the FM phase of FCC Fe. On the whole, all workers [6–8] point out that, for FM FCC Fe, two states with only slightly different energies exist in the discussed interval of atomic volumes: LS at low volumes and the HS at high volumes. The presence of these states plays an important role in the Invar effects in Fe–Ni alloys [9].

In [6, 8] the volume dependence of the local magnetic moment has been investigated for the AFM configuration too. All calculations have shown the existence of only one spin state for AFM FCC Fe over a considerable range of crystal volume expansions. The

magnetic moments of this state increase continuously with increasing volume expansion (see figure 1). As figure 1 shows, our results for $q = 0$, $q = 1$ are in accordance with those for FM and AFM FCC Fe [6, 8].

The analysis of the q -dependence of $m(q)$ functions shows that, at small q ($q \leq 0.5$), the function $m(q)$ for $S = 2.66$ au differs substantially from that for $S = 2.69, 2.72$ and 2.78 au. At the same time for $q \approx 1$ the dependences of the $m(q)$ -function on q are quite similar for all volumes. This behaviour of the $m(q)$ -function results from the fact that two magnetic states exist in FM FCC Fe and only one magnetic state in AFM FCC Fe for all volumes studied. So at $S = 2.69, 2.72$ and 2.78 au the variation in q from 0 to 1 leads to continuous transformations of the HS state for FM FCC Fe into the only state of AFM FCC Fe. Thus we can suppose that the stable AFM state is connected 'genetically' with the HS state of FM FCC Fe, whereas for $S = 2.66$ au the spiral states with small q up to $q = 0.5$ are connected 'genetically' with the LS state of FM FCC Fe. For $q > 0.5$, the nature of the states corresponding to the minimum of total energy is changed and these states are connected with only the one magnetic state of AFM FCC Fe.

Figure 2 shows the results of the self-consistent total energy calculations $E(q)$ as functions of magnitude of spin-spiral vector q . For Wigner-Seitz radii $S = 2.66, 2.69$ and 2.72 au the minimum of the $E(q)$ -function corresponds to a SSDW. This result is consistent with experimental data [4]. It agrees also with the theoretical estimations in [11] where the existence of the stable spiral structure in FCC Fe was predicted on the basis of the calculations of the unenhanced magnetic susceptibility. The position of the $E(q)$ -minimum at an intermediate value of q is the most clearly expressed for $S = 2.72$ au (figure 2). There is a tendency for the difference between the energy of the minimum $E(q)$ -function and the energy of the AFM state to decrease with decrease in volume. Note that for a Wigner-Seitz radius of $S = 2.66$ au, the AFM configuration has a lower energy than the FM configuration. The differences between the total energies of AFM and FM configurations change sign as S increases (figure 2). Thus there is tendency

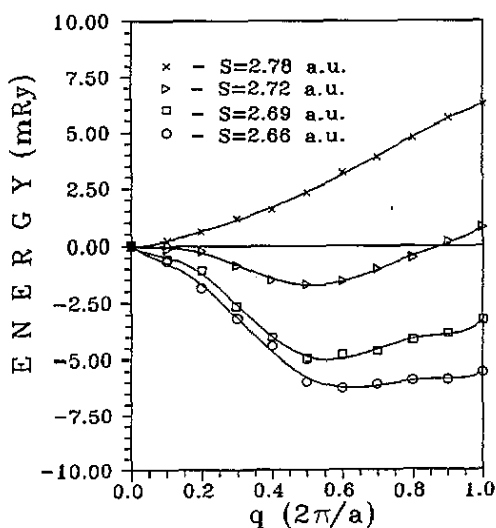


Figure 2. The total energy of the spin-spiral magnetic configurations relative to that of the ferromagnetic state for FCC Fe.

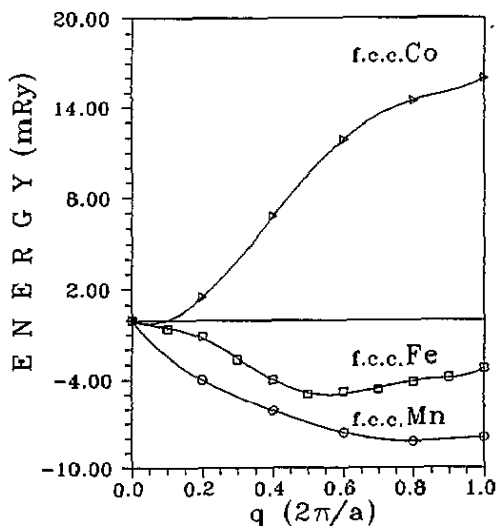


Figure 3. The total energy of the SSDWs relative to that of the ferromagnetic state for FCC Co, Fe and Mn.

towards the formation of the FM HS state for larger S (2.78 au). At the same time for the LS state there is tendency for non-collinear AFM ordering. This conclusion is in accordance with experimental observations that FCC Fe precipitates in Cu–Au alloys ($S = 2.78$ au) are FM [2] and FCC Fe precipitates in Cu ($S = 2.67$ au) are AFM [3] and with the results of the previous calculations on FM and AFM FCC Fe [6–8] but contradicting the result in [10].

In order to study the dependence of the position of the $E(q)$ -minimum on the number of valence electrons we have carried out calculations for FCC Co, Fe and Mn with the same Wigner–Seitz radius $S = 2.69$ au. The results (figure 3) indicate that the increase in the number of valence electrons tends to stabilize ferromagnetic ordering (FCC Co). This result is in agreement with experimental data [20]. The opposite tendency is observed with a decreasing number of valence electrons. The minimum of the $E(q)$ -function for FCC Mn shifts to an AFM configuration. This property is in accordance with the phase diagram obtained in [21]. Thus, our results confirm the conclusion of [21] that, in the magnetic phase diagram of 3d metals with FCC lattices, Fe is located at a crossing point between the regions of FM and AFM ordering.

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