(§ 3) reaches saturation only when the magnetic pressure becomes comparable with the plasma pressure. Let us assume that initially we have $\beta \ll 1$ (low-pressure plasma). According to Eq. (16) the value of $\langle H^2 \rangle$ increases proportionally to ρ, whereas $p \propto \rho^{\gamma}$ in the case of adiabatic compression (γ is the specific heat ratio). Since $\gamma > 1$, the plasma pressure finally prevents compression. Consequently, a turbulent medium acquires regions with a much higher local pressure.

4. The nonpotential forces acting on a plasma appear because of the anisotropy (§ 1) or are manifested as a negative resistance [§ 4, Eq. (27)]. Large-scale flow may be produced in a plasma under the action of these forces. By way of example, we shall mention the excitation of shear motion in the solar wind because of the inhomogeneity of $\langle H^2 \rangle$ and a possible anisotropy of the magnetic inhomogeneities.

The author is grateful to A. A. Vedenov, V. D. Shapiro, and V. I. Shevchenko for reviewing the results and valuable discussions.

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Translated by A. Tybulewicz

Magnetic moments of iron atoms in the fcc lattice of a transition *d*-metal

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(Submitted 26 July 1978)
Zh. Eksp. Teor. Fiz. **74**, 2066–2077 (June 1978)

The atomic magnetic moment m_{Fe} was investigated in the fcc modification of iron (the γ phase) and in its alloys with transition d-metals. The behavior of m_{Fe} was investigated as a function of the integral V of the transition between the localized levels of neighboring atoms at a fixed value of the mixing constant of the s and d states. In the assumed model, the magnetic state of the atom is determined only by the influence of its nearest neighbors. It is shown that the atomic magnetic moment of γ-iron decreases with increasing V. At $V \approx 0.35$ eV, m_{Fe} vanishes, but in the same region of V the value of m_{Fe} for the bcc modification of iron changes insignificantly. The function $m_{\mathrm{Fe}}(V)$ for γ-Fe is considered with allowance for the transition of the conduction electrons to localized levels as V increases. It is shown that m_{Fe} of impurity iron atoms in d-metals with fcc lattices depends on the quantity E_{Fe}^{-} and E_{M}^{-}, where E_{Fe}^{-} is the energy of the d level of the iron atom at $V = 0$ with a spin direction corresponding to the less occupied part of this level, and E_{M}^{-} is the analogous quantity for the matrix atoms. If the condition $E_{\mathrm{Fe}}^{-} - E_{\mathrm{M}}^{-} > 4V$ is satisfied, then m_{Fe} of the impurity iron atoms depends little on V. This conclusion explains why impurity iron atoms in many d-metals with fcc lattice have large and approximately equal values of m_{Fe}, equal to (2.5–3) μ_B, whereas γ-Fe has a small atomic magnetic moment, (0.5–0.7) μ_B. The dependence of the mean value $\bar{m}_{\mathrm{Fe}}$ on the iron concentration in alloys with d-metals having an fcc lattice is considered. In accord with the experimental data, the obtained relation $\bar{m}_{\mathrm{Fe}}(c)$ tends rapidly to zero at a certain critical iron concentration c_{cr}.

PACS numbers: 75.50.Bb, 35.10.Di

INTRODUCTION

The magnetic properties of iron in the face-centered cubic (fcc) modification (γ phase) differ strongly from the properties of its usual body-centered cubic (bcc) modifications (α phase). Iron in the γ modification is antiferromagnetic. Its atomic magnetic moment is $(0.7-0.5)\mu_B$,[1,2] much higher than the atomic magnetic moment $2.2\mu_B$ of α iron. In the fcc lattice of transition d-metals, however, impurity iron atoms have relatively large spin magnetic moments that vary over a small range, approximately from $2.5\mu_B$ to $3\mu_B$ for different matrices. Magnetic moments of this order are possessed by alloys based on Ag[3]; Au[4,5]; Co[6]; Cu[7]; Ni[8,5]; Pd[9]; Pt.[10] These alloys are either ferromagnets or paramagnets.

The magnetic properties of the iron atoms vary strongly in alloys based on γ iron. In the fcc alloys FeCrNi (stainless steel) and FeMn the magnetic mo-

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ment of the iron atoms is only $(0.3-0.5)\mu_B$.[2, 11] These alloys are antiferromagnetic.[12, 13]

Thus, iron atoms can be in two different magnetic states in the fcc lattice of a d-metal. This circumstance was first noted by Tauer and Weiss.[14, 15] The process of the transition of the iron atoms from a state with large magnetic moment to a state with a small magnetic moment is observed in certain disordered alloys when the iron concentration is increased. A classical system in this respect is made up of the γ-FeNi alloys. At low iron concentrations the total magnetic moment of these ferromagnetic alloys is made up almost additively of the atomic moments of nickel $(0.6\mu_B)$ and iron $(2.8\mu_B)$.[16] When the nickel content is decreased below 40%, the spontaneous magnetization begins to decrease rapidly with increasing iron concentration. This decrease is the result of the change of the magnetic state of a fraction of the iron atoms in the γ-FeNi alloys.[17, 18, 19, 20] At a large iron content in these alloys, however, the γ phase becomes unstable at low temperatures. It is therefore impossible to trace directly the change produced in the magnetic properties of γ-FeNi alloys by a change of the magnetic states of all the iron atoms in the alloy.

The pattern of the transformation of the magnetic properties of individual iron atoms in the fcc lattice as they interact with one another can be most clearly traced with CuFe alloys as an example. The iron can form a solid dilute solution in the copper, or else exist in the copper lattice in the form of clusters or segregations of γ-Fe. The CuFe alloys constitute therefore a convenient system for the study of the magnetic properties of isolated iron atoms and their complexes. The states of the iron atoms in CuFe we investigated experimentally with the aid of the Mössbauer effect,[21, 22] nuclear magnetic resonance,[23] as well as magnetic measurements.[7] The results of these investigations have shown that when the iron atoms are completely surrounded by copper atoms they have a localized magnetic moment equal of $2.5\mu_B$. If the nearest neighbors of these atoms include a small number of other iron atoms, their magnetic moment does not change substantially. But if the number of nearest neighbors of the Fe-Fe type is large enough, the iron atoms lose their magnetic moment. To interpret this effect we must call attention to the following facts.

1) The crystal-lattice constant of copper is very close to that of γ-Fe, being 3.616 Å for the former and 3.588 Å for the latter.[24]

2) Impurity iron atoms in a copper matrix are in a $3d^7 4s^1$ state.[23]

3) The partition of the electrons between the $3d$ and $4s$ bands of γ iron also corresponds to the $3d^7 4s^1$ configuration. This statement follows from theoretical calculations of the electron structure of γ-Fe.[25, 26] In addition, this conclusion is confirmed by results of investigations of the positron annihilation in alloys based on γ-Fe.[27] It should be noted that the $3d^7 4s^1$ configuration is also realized in the usual ferromagnetic α modification of iron.[28]

The arguments advanced in items 1)–3) above give grounds for assuming that replacement of the copper atoms surrounding the iron atom in question by other iron atoms is equivalent to turning on a d–d interaction between them. The most significant part of this interaction is connected with "hopping" of the electrons between d levels of neighboring atoms.[29]

Experiments (see[19–22]) show that the principal effect is exerted on the value of the localized atomic magnetic moment of iron by its nearest neighbors. This conclusion holds true also for the atomic magnetic moments and for other transition d-metals.[30, 31] Thus, the analysis of the effect of interatomic transitions on the magnetic state of the atom can be confined to the first coordination sphere. This paper deals with the influence of this effect on the localized spin magnetic moments of an iron atom in an fcc lattice of a d-metal.

1. THE HAMILTONIAN

We assume that the atomic magnetic moments of the considered d-metals have the same nature as the impurity magnetic moments in Anderson's theory.[32] This approach to the description of ferromagnetic d-metals was first used in.[29, 33] In this model the atomic magnetic moment depends on the overlap of the d-wave functions of the neighboring atoms.

We assume also that the atomic magnetic moments are the result of the existence of only one state localized in the atom.

The Hamiltonian for this model is of the form

$$H=\sum_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k}}^{\sigma}a_{\mathbf{k}\sigma}^{+}a_{\mathbf{k}\sigma}+\sum_{i\sigma}E_i^0 a_{i\sigma}^{+}a_{i\sigma}+\sum_i U_i a_{i\sigma}^{+}a_{i\sigma}a_{i-\sigma}^{+}a_{i-\sigma}$$
$$+\sum_{\mathbf{k}i\sigma}(V_{\mathbf{k}i}a_{\mathbf{k}\sigma}^{+}a_{i\sigma}+V_{i\mathbf{k}}a_{i\sigma}^{+}a_{\mathbf{k}\sigma})+\sum_{i\neq j\sigma}V_{ij}a_{i\sigma}^{+}a_{j\sigma}. \tag{1.1}$$

The symbols in this expression are standard. The first term of (1.1) describes the kinetic energy of the conduction electrons, E_i^0 is the energy of the localized state in the field of the i-th ion and in the intracrystalline field. The third term determines the spin-splitting energy of the localized states as a result of the intra-atomic interaction characterized by the constant U_i. In the Hartree-Fock approximation, as a result of this interaction, the energy of the localized state turns out to be

$$E_i^{\sigma}=E_i^0+U_i n_i^{-\sigma}, \tag{1.2}$$

where n_i^{σ} is the average occupation number of the electron level with spin σ, localized in the i-th site. The fourth and fifth terms of (1.1) describe the s–d and d–d mixing; V_{ki} is the integral of the transition between the s and d states:

$$V_{\mathbf{k}i}=\int\varphi_{\mathbf{k}}^{*}(\mathbf{r})v_i(\mathbf{r})\psi_i(\mathbf{r})d^3\mathbf{r}, \tag{1.3}$$

where $\varphi_k^*(\mathbf{r})$ and $\varphi_i(\mathbf{r})$ are the wave functions of the s and d electrons, and $v_i(\mathbf{r})$ is the effective potential of the ion located in site i. The quantity V_{ij} is the integral of the transition between the localized states of the neighboring sites i and j.

2. GREEN'S FUNCTION OF THE LOCALIZED STATE

It is convenient to calculate the localized magnetic moments in a system with Hamiltonian (1.1) with the aid of Green's functions, using the equations[32]

$$n_i^\sigma = \frac{-1}{\pi} \int\limits_{-\infty}^{\varepsilon_F} \operatorname{Im} G_{ii}^\sigma(\varepsilon)\, d\varepsilon. \qquad (2.1)$$

Here $G_{ii}^\sigma(\epsilon)$ is the Green's function for a state localized at site i. The integration with respect to ϵ in (2.1) is carried out up to the Fermi level ϵ_F. We can write in general form

$$G_{ii}^\sigma(\varepsilon) = \frac{1}{\varepsilon - E_i^\sigma - M_i^\sigma(\varepsilon)}, \qquad (2.2)$$

where $M_i^\sigma(\epsilon)$ is the mass operator that takes into account the interaction of the i-th atom with the surrounding medium. We represent the expression for the mass operator in the form of two terms that describe different physical processes:

$$M_i^\sigma(\varepsilon) = M_{i1}^\sigma(\varepsilon) + M_{i2}^\sigma(\varepsilon) \qquad (2.3)$$

The first term in the right-hand side of (2.3) takes into account the interaction of the level localized in site i with the conduction-band levels. The second term is connected with the d–d interaction between the i-th atoms and the remaining lattice sites. If we start with the Hamiltonian (1.1), then the expression for $M_{i1}^\sigma(\epsilon)$ takes the form[34]

$$M_{i1}^\sigma(\varepsilon) = \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}i}|^2}{\varepsilon - \varepsilon_{\mathbf{k}}^\sigma + i\delta}. \qquad (2.4)$$

This function has nonzero real and imaginary parts, so that

$$M_{i1}^\sigma(\varepsilon) = \Delta_i^\sigma(\varepsilon) - i\Gamma_i^\sigma(\varepsilon). \qquad (2.5)$$

It follows from (2.4) that the imaginary part of M_{i1}^σ is

$$\Gamma_i^\sigma(\varepsilon) = \pi\rho_s^\sigma(\varepsilon)\,[\,|V_{ik}|^2]_\varepsilon, \qquad (2.6)$$

where $\rho_s^\sigma(\epsilon)$ is the conduction-electron density distribution function. The square brackets with the subscript ϵ indicate that $\mathbf{k}$ corresponds to $\epsilon_{\mathbf{k}}$ equal to ϵ.

When indirect-interaction effects are disregarded, M_{i2}^σ can be represented by the following series[35]:

$$M_{i2}^\sigma(\varepsilon) = \sum_{j \neq i} \frac{V_{ij}V_{ji}}{\varepsilon - E_j^\sigma + i\delta} + \sum_{j \neq i;\, k \neq i,j} \frac{V_{ij}V_{jk}V_{ki}}{(\varepsilon - E_j^\sigma + i\delta)(\varepsilon - E_k^\sigma + i\delta)} + \dots \qquad (2.7)$$

In this expression, the summation corresponds to all the electron trajectories that begin and end with the i-th site. These trajectories pass through the surrounding atoms in all possible ways.

In the case of a pure metal we assume that $V_{jl} = V$ if j and l are nearest neighbors. For sites that are not nearest neighbors, $V_{jl} = 0$. In addition, for a pure metal with ferromagnetically arranged atomic magnetic moments the quantity $E_j^\sigma + M_{ij}^\sigma(\epsilon)$ does not depend on the subscript l. Taking these remarks into account, we can represent the aggregate of those terms in expression (2.7) for $M_{i2}^\sigma(\epsilon)$ which pertain only to the first coordination sphere, in the case of an fcc lattice, by the series

$$\frac{12V^2}{\varepsilon - E^\sigma - M_1^\sigma(\varepsilon)} \left[1 + \frac{4V}{\varepsilon - E^\sigma - M_1^\sigma(\varepsilon)} + \left(\frac{4V}{\varepsilon - E^\sigma - M_1^\sigma(\varepsilon)}\right)^2 + \dots\right]. \qquad (2.8)$$

This expression takes account of the fact that each site of the first coordination sphere includes among its nearest neighbors four sites that are contained in the coordination sphere in question.

The complete expression for $M_2^\sigma(\epsilon)$ is the series

$$M_2^\sigma(\varepsilon) = V \sum_{n=1}^{\infty} C_n [\lambda^\sigma(\varepsilon)]^n, \qquad (2.9)$$

where

$$\lambda^\sigma(\varepsilon) = \frac{V}{\varepsilon - E^\sigma - M_1^\sigma(\varepsilon)}. \qquad (2.10)$$

The coefficients C_n are constants that depend only on the lattice symmetry.

The contribution made to (2.9) by the second, third, and fourth coordination spheres begins with terms proportional to $(\lambda^\sigma)^3$. The more remote coordination spheres contribute only to the terms containing λ^σ raised to higher powers. It is obvious that with decreasing $|\lambda^\sigma|$ the relative role of the nearby coordination spheres increases in expression (2.9) for $M_2^\sigma(\epsilon)$. The quantiy $\Gamma^\sigma(\epsilon)$ in (2.5) is usually approximated by a constant Γ that characterizes the virtual width of the energy level. In this case the maximum value of $|\lambda^\sigma|$ is V/Γ. For real metals this ratio is much less than unity.

According to (2.8), the expression for $M_2^\sigma(\epsilon)$, when account is taken of only the first coordination sphere, takes the form

$$M_2^\sigma(\varepsilon) = \frac{12V^2}{\varepsilon - E^\sigma - M_1^\sigma(\varepsilon) - 4V}. \qquad (2.11)$$

This expression takes exact account of the terms proportional to λ^σ and $(\lambda^\sigma)^2$ of the series (2.9). In this approximation, if $M_1^\sigma(\epsilon)$ is constant, the function $G_{ii}^\sigma(\epsilon)$ has only two poles. In the general case, when account is taken of all the terms in expression (2.9) for $M_2^\sigma(\epsilon)$, the number of poles of $G_{ii}^\sigma(\epsilon)$ is equal to the number of energy levels in the corresponding band; then

$$G_{ii}^\sigma(\varepsilon) = \frac{1}{N} \sum_{\mathbf{k}} G^\sigma(\varepsilon, \mathbf{k}), \qquad (2.12)$$

where $G^\sigma(\epsilon, \mathbf{k})$ is the one-electron Green's function in the quasimomentum representation and N is the number of atoms in the system under consideration.

3. EQUATIONS FOR THE DETERMINATION OF THE ATOMIC MAGNETIC MOMENT

The localized magnetic moment m_i of an atom located at site i is equal to

$$m_i = 5(n_i^+ - n_i^-)\,\mu_B. \qquad (3.1)$$

The factor 5 arises as a result of five-fold degeneracy of the localized d level. The subscript i will be omitted from now on. The average occupation numbers n^σ are determined by two equations (2.1) corresponding to two values of σ. These equations become much simpler if $M_1^\sigma(\epsilon)$ is taken to be constant.

This approximation leads to the same main conclusions concerning the properties of the localized magnetic moments.[32, 34] In addition, we assume that $M_1^+ = M_1^-$. This condition presupposes the absence of spin splitting of the states in the conduction band. Under the indicated assumptions, with allowance for expression (2.11) for $M_2^\sigma(\epsilon)$, the equations (2.1) for n^σ take the form

$$n^\sigma = -\frac{1}{\pi}\,\mathrm{Im}\int_{-\infty}^{\varepsilon_F} \frac{d\varepsilon}{\varepsilon - E^\sigma - \Delta + i\Gamma - 12V^2/(\varepsilon - E^\sigma - \Delta + i\Gamma - 4V)}. \tag{3.2}$$

The integral in the right-hand side of this equation can be calculated in explicit form. As a result of the integration we obtain the following equations for n^σ:

$$n^\sigma = \frac{1}{4\pi}\left\{3\,\mathrm{arcctg}\left(\frac{E^\sigma + \Delta - 2V - \varepsilon_F}{\Gamma}\right) + \mathrm{arcctg}\left(\frac{E^\sigma + \Delta + 6V - \varepsilon_F}{\Gamma}\right)\right\}, \tag{3.3}$$

where $E^\sigma = E^0 + Un^{-\sigma}$. The function $\tan^{-1} x$ in these equations ranges from zero to π.

To elucidate the physical meaning of (3.3), we must consider the effect of V on the local density of states $\rho_i^\sigma(\epsilon, V)$:

$$\rho_i^\sigma(\varepsilon, V) = -\frac{1}{\pi}\,\mathrm{Im}\,G_{ii}^\sigma(\varepsilon, V). \tag{3.4}$$

If there is no interaction between the atoms, the local density of states has only one peak, whose shape is described by the expression

$$\rho^\sigma(\varepsilon, 0) = \frac{1}{\pi}\,\frac{\Gamma}{(\varepsilon - E^\sigma - \Delta)^2 + \Gamma^2}. \tag{3.5}$$

When account is taken of the interatomic interaction in the employed approximation, $\rho^\sigma(\epsilon, V)$ splits into two unequal parts, $\rho_1^\sigma(\epsilon, V)$ and $\rho_2^\sigma(\epsilon, V)$. The maxima of ρ_1^σ and ρ_2^σ occur at the respective values

$$\varepsilon_1^\sigma = E^\sigma + \Delta - 2V, \quad \varepsilon_2^\sigma = E^\sigma + \Delta + 6V. \tag{3.6}$$

The distance between the maxima of ρ_1^σ and ρ_2^σ is $\epsilon_2^\sigma - \epsilon_1^\sigma = 8V$. If V is equal to several tenths of an electron volt, the value of $\epsilon_2^\sigma - \epsilon_1^\sigma$ is of the order of the energy width of the $3d$ band of iron. The two terms in the right-hand side of (3.3) are the occupation numbers of the levels corresponding to ρ_1^σ and ρ_2^σ.

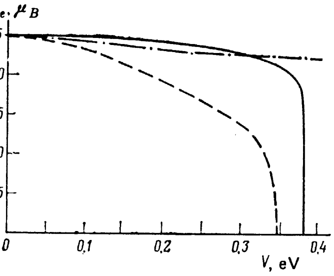

FIG. 1. Dependence of the atomic magnetic moment m_{Fe} for the fcc and bcc modifications of iron on the transition integral V. The dashed line corresponds to a constant Fermi energy ϵ_F in the case of an fcc lattice. The dash-dot line is the analogous plot for the bcc lattice. The solid line describes the function $m_{Fe}(V)$ for the fcc modification of iron with allowance for the $\epsilon_F(V)$ dependence that results from the transition of some of the conduction electrons to d levels with increasing V.

We note that the splitting of the local state density of the magnetic atoms under the influence of their nearest neighbors was pointed out in,[30] where the effect of the nearest neighborhoods on the atomic magnetic moment of the central atom was treated by the methods of the coherent-potential theory.

The constants $E^0 + \Delta - \epsilon_F$ and U can be determined by using the experimental results. According to[23], for an iron impurity atom in copper we have $n^+ = 0.95$, $n^- = 0.45$, and $\Gamma = 0.71$ eV. If it is assumed that $V = 0$ in this case, then it follows from (3.3) that $E^0 + \Delta - \epsilon_F = -8.62$ eV and $U = 9.19$ eV. For these values of the constants $E^0 + \Delta - \epsilon_F$ and U, Eqs. (3.3) were solved numerically for different values of V. The values of m_{Fe} obtained in this manner as functions of V are shown by the dashed line of Fig. 1. As seen from this plot, the value of m_{Fe} calculated with the aid of Eqs. (3.3) vanishes when V exceeds approximately 0.35 eV. The value of V for γ-iron can be estimated from the band width[29, 33] by using the relation

$$\Delta E = 2zV, \tag{3.7}$$

where ΔE is the width of the band and z is the number of nearest neighbors. According to the results of the calculations of the band structure of γ iron,[25,36] the value of V for this modification of iron is approximately 0.25 eV. The estimate of V with the aid of (3.7) is, however, a crude one.

The physical causes of the decrease of m_{Fe} with increasing V are the following. When there is no interaction between the atoms, the energy $3d$ level of the iron atom with negative spin direction ($n^- < n^+$) lies near the Fermi level ($E^- + \Delta - \epsilon_F = 0.11$ eV). When the interatomic interaction is turned on, $\rho^-(\epsilon, V)$ splits into two unequal parts. That part of the initial level which has the larger capacity drops below the Fermi level. As a result, the number n^- increases. The increase of n^- leads to a decrease of the intra-atomic splitting and accordingly to a decrease of n^+. This process leads to a decrease of m_{Fe}.

Calculations show that the sum of the values of n^+ and n^- satisfying Eqs. (3.3) does not remain constant when V is varied. In the region of V where m_{Fe} tends to zero, $n^+ + n^-$ increases by approximately 10%. This change of $n^+ + n^-$ is due to the transition of the conduction electrons to localized levels with increasing V. In the real case the d level has 5 orbital states. Therefore an appreciable part of the $4s$ electrons in γ-iron should go over to the $3d$ levels, owing to the interaction between the localized electrons of the neighboring sites. It is therefore necessary to take the dependence of ϵ_F on $n^+(V) + n^-(V)$ into account in the initial equations (3.3) for n^σ.

In the case of the simplest dispersion law for the conduction electrons, when $\epsilon_F = \hbar^2 \mathbf{k}^2/2m$, the expression that takes the $\epsilon_F(V)$ dependence into account is of the form

$$\varepsilon_F(V) = \varepsilon_F(0)\left[1 - 5\,\frac{n^+(V) + n^-(V) - n^+(0) - n^-(0)}{n_s(0)}\right]^{2/3}, \tag{3.8}$$

where $n_s(0)$ is the average number of 4*s* electrons per atom. As already noted in the Introduction, the experiment described in[23] shows that the impurity atoms of iron in copper (the case $V = 0$) are in a state with configuration $3d^4 4s^1$. We shall therefore assume that $n_s(0) = 1$. Accordingly, we set $\epsilon_F(0)$ equal to the Fermi energy of copper. In the employed approximation, this quantity is equal to 7.42 eV.[34] The factor 5 in expression (3.8) takes into account the existence of orbital states for the *d* level.

The values of m_{Fe} as functions of V, with allowance for the $\epsilon_F(V)$ dependence in Eqs. (3.3), are shown in Fig. 1 by the solid line. A characteristic feature of this curve is that m_{Fe} varies little in a wide range of V, approximately from zero to 0.35 eV, and drops steeply to zero near 0.38 eV. In addition, allowance for the $\epsilon_F(V)$ dependence causes $n^+ + n^-$ to remain constant within 2% with changing V. The last result agrees with the conclusion[27] that the γ-iron atoms are in a state with configuration $3d^7 4s^1$.

The equations for the occupation numbers n^σ in the case of a bcc lattice differ from Eqs. (3.3) for the fcc lattice. The difference is due to two causes. First, the numbers of the nearest neighbors of the bcc and fcc lattice sites are different and equal 8 and 12, respectively. Second, the coefficient $C_2 = 0$ in expression (2.9) for $M_2^\sigma(\epsilon)$ for the bcc lattice. In this case, if account is taken of only the first coordination sphere,

$$M_2^\sigma(\varepsilon) = \frac{8V^2}{\varepsilon - E^\sigma - M_1(\varepsilon)}. \tag{3.9}$$

In this approximation, the equations for n^σ take the form

$$n^\sigma = \frac{1}{2\pi}\left\{\operatorname{arcctg}\left(\frac{E^\sigma + \Delta - V\sqrt{8} - \varepsilon_F}{\Gamma}\right) + \operatorname{arcctg}\left(\frac{E^\sigma + \Delta + V\sqrt{8} - \varepsilon_F}{\Gamma}\right)\right. \tag{3.10}$$

The values of m_{Fe} for the bcc lattice, determined from Eqs. (3.10) are shown in Fig. 1 by the dash-dot line. In the calculation of these m_{Fe}, the values of $E^0 + \Delta - \epsilon_F$ and U were taken to be the same as in the case of γ-Fe. As seen from Fig. 1, the magnetic moment for α-Fe depends little on the value of V in the region of V that is of physical interest.

4. MAGNETIC MOMENT OF THE IRON ATOMS IN ALLOYS

In Anderson's theory[32] the localized impurity moment depends only on the internal properties of the impurity atom and on the *s–d* interaction. Experiments[19, 22] show, however, that magnetic moments of the impurities depend substantially on the properties of their nearest-neighbor atoms. This effect can be interpreted by taking the interatomic transitions into account. In the employed approximation the Green's function of the impurity atom takes the form

$$G^\sigma_{\text{imp,imp}}(\varepsilon) = [\varepsilon - E_{\text{п}}^\sigma + i\Gamma - 12V^2/(\varepsilon - E_{\text{M}}^\sigma + i\Gamma - 4V)]^{-1}, \tag{4.1}$$

where E^σ_{imp} and E^σ_{M} are respectively the *d*-level energies of the isolated impurity and matrix atoms. It is assumed in (4.1) that the transition integral $V_{i,j}$ does not depend on the type of the atoms situated in the sites *i* and *j*. The virtual widths of the localized levels of the impurity and matrix atoms are assumed to be the same and equal to Γ. In addition, the atomic-level shifts due to the *s–d* mixing are also assumed to be the same for the impurity and matrix atoms. The quantity Δ is included in E^σ_{imp} and E^σ_{M}. The impurity-atom local state density $\rho^\sigma_{\text{imp}}(\epsilon, V)$, which corresponds to the Green's function (4.1), is equal to

$$\rho_{\text{imp}}^\sigma(\varepsilon, V) = \frac{\Gamma}{2\pi}\left\{\left(1 + \frac{A_\sigma}{(A_\sigma^2 + 48V^2)^{1/2}}\right)\frac{1}{(\varepsilon - \varepsilon_1^\sigma)^2 + \Gamma^2} + \left(1 - \frac{A_\sigma}{(A_\sigma^2 + 48V^2)^{1/2}}\right)\frac{1}{(\varepsilon - \varepsilon_2^\sigma)^2 + \Gamma^2}\right\}, \tag{4.2}$$

where

$$A_\sigma = E_{\text{imp}}^\sigma - E_{\text{imp}}^\sigma - 4V,$$
$$\varepsilon_{1,2}^\sigma = {}^1/_2\{E_{\text{imp}}^\sigma + E_{\text{M}}^\sigma + 4V \pm (A_\sigma^2 + 48V^2)^{1/2}\}. \tag{4.3}$$

If $V = 0$ then, as follows from (4.2), $\rho^\sigma_{\text{imp}}(\epsilon, 0)$ has only one peak, whose maximum is located at $\epsilon = E^\sigma_{\text{imp}}$. Its shape is described by the Lorentz curve (3.5). Under the influence of V, the local state density of the impurity atom splits into two parts corresponding to the two terms of (4.2). The positions of the maxima of these parts, as well as their intensities, depend on V, E^σ_{imp}, and E^σ_{M}.

As already noted in Sec. 3, the decrease of m_{Fe} with increasing V is physically due mainly to the character of splitting of $\rho^-(\epsilon, V)$, since the maximum of $\rho^-(\epsilon, 0)$ for iron lies near the Fermi level. To draw general conclusions concerning the influence of the matrix on the value of m_{Fe} of the impurity iron atom it is therefore sufficient to consider the pattern of the splitting of $\rho^-_{\text{imp}}(\epsilon, V)$.

If $E^-_{\text{imp}} - E^-_{\text{M}} > 4V$, i.e. $A_- > 0$, the the more intense part of $\rho^-_{\text{imp}}(\epsilon, V)$ corresponds to the first term in (4.2). The value of ϵ_1^- increases with increasing V. Thus, if the *d* level of the matrix atoms with negative spin direction lies below the corresponding level of the impurity atom and the condition $E^-_{\text{imp}} - E^-_{\text{M}} \gg 4V$ is satisfied, then m_{Fe} does not decrease when V is increased.

If $E^-_{\text{imp}} - E^-_{\text{M}} < 4V$, then the more intense peak corresponds to the second term in expression (4.2) for ρ^- (ϵ, V). In this case m can decrease with increasing V. At sufficiently rare absolute values of $E^-_{\text{Fe}} - E_M$, when the condition $(E^-_{\text{imp}} - E^-_{\text{M}} - \text{eV})^2 \gg 48V^2$ is satisfied, the effect of the matrix on the localized level of the impurity atom becomes weak.

As already noted in the Introduction, the lattice parameters and the conduction-electron concentrations of copper and of γ-Fe are close to each other. Therefore the appreciable difference between the values of the impurity moment of iron in copper and of the atomic magnetic moment of γ-Fe must be attributed to the difference in the character of the *d–d* interactions in these two cases. The 3*d* band of copper is completely filled, so that $E^-_{\text{Fe}} - E^-_{\text{Cu}} > 0$. It must be concluded from the experimental and theoretical data[37] that $E^-_{\text{Fe}} - E^-_{\text{Cu}} \approx 3-4$ eV. Thus, the condition under which the iron impurity atom retains a large moment is satisfied in this case.

For the remaining transition metals listed in the Introduction and in which iron is dissolved, the d band is either likewise completely filled, or else contains a larger number of electrons per atom than the d level of the iron impurity atom. The condition $E^{-}_{\mathrm{imp}}-E^{-}_{\mathrm{M}}>0$ is therefore satisfied also for these metals and contributes to the conservation of the impurity magnetic moment of the iron.

In concentrated iron alloys, the individual iron atoms have different values of m_{Fe}, depending on the concrete form of the distribution of the alloy-component atoms around them. The character of the influence of the iron and of the second component of the alloy on the m_{Fe} of the introduced atoms is in general different. The average atomic magnetic moment $\bar{m}_{\mathrm{Fe}}$ of the iron atoms in the allov is therefore a function of the alloy composition.

To gain a general idea of the $\bar{m}_{\mathrm{Fe}}(c)$ dependence, we make a number of assumptions that simplify the determination of this function. We assume that for the second component in the iron alloy the condition $(E^{-}_{\mathrm{imp}}=-E^{-}_{\mathrm{M}}-4V)^2\gg 48V^2$ is satisfied, i.e., that the atoms of this component exert no significant influence on m_{Fe}. We need therefore retain in the general expression (2.7) for M_2^σ only those terms that pertain to the lattice sites occupied by the iron atoms. To calculate the average atomic moment $\bar{m}_{\mathrm{Fe}}$ we determine next, with the aid of (2.1), the mass operator $\bar{M}_2^\sigma(\epsilon, c)$. It is necessary for this purpose to take into account the probability of the iron occupying the individual lattice sites. We sum in (2.7) not only over the sites occupied by iron atoms, but over all the lattice sites, but each summation sign in (2.7) will be supplemented by an additional factor c equal to the iron concentration. In this approximation, the mean value $\bar{M}_2^\sigma(\epsilon, c)$ determined in this manner is

$$\bar{M}_2^\sigma(\epsilon, c)=12V^2c/(\epsilon-E^\sigma-M_1-4Vc). \tag{4.4}$$

With this approximation, Eqs. (2.1) for $\bar{m}_{\mathrm{Fe}}$ take the form

$$\bar{n}^\sigma=\frac{1}{2\pi}\frac{1}{(c^2+3c)^{1/2}}\left\{[c+(c^2+3c)^{1/2}]\operatorname{arcctg}\left[\frac{\bar{E}^\sigma+\Delta+2V(c-(c^2+3c)^{1/2})-\varepsilon_F}{\Gamma}\right]\right.$$
$$\left.-[c-(c^2+3c)^{1/2}]\operatorname{arcctg}\left(\frac{\bar{E}^\sigma+\Delta+2V(c+(c^2+3c)^{1/2})-\varepsilon_F}{\Gamma}\right)\right\}. \tag{4.5}$$

At $c=1$ these equations go over into the initial expressions (3.3), and at $c=0$ Eqs. (4.5) coincide with the usual Anderson equations.[32]

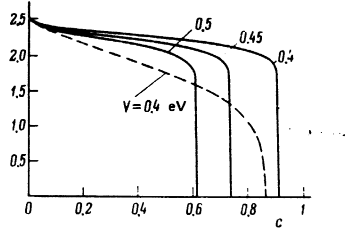

FIG. 2. Plots of the average magnetic moment $\bar{m}_{\mathrm{Fe}}$ against the iron concentration c in alloys having an fcc lattice at different constant values of V. The dashed line corresponds to a constant Fermi energy ϵ_F. The solid lines take into account the $\epsilon_F(c)$ dependence resulting from the transition of some of the conduction electrons to the d levels with increasing c.

The dashed line in Fig. 2 shows a plot of $\bar{m}_{\mathrm{Fe}}$ against the concentration c of the iron in the alloy for the case $V=0.4$ eV. This $\bar{m}_{\mathrm{Fe}}(c)$ dependence is determined with the aid of Eqs. (4.5), in which ϵ_F is assumed constant. In this case, when c is varied, the occupation numbers n^+ and n^-, which are solutions of Eqs. (4.5), do not leave the quantity $n^+ + n^-$ constant. Therefore, an analogy with the solution of Eqs. (3.3) for pure γ-Fe, it is likewise necessary in this case to take into account the changes of the conduction-electron concentration. Allowance for this effect leads to replacement of E_F in (4.5) by $\epsilon_F(c)$:

$$\varepsilon_F(c)=\varepsilon_F(0)[1-5c(n^+(c)+n^-(c)-1.4)]^{2/3}, \tag{4.6}$$

where $n^+(0)+n^-(0)=1.4$. Expression (4.6) presupposes that as $c\to 0$ the concentration of the conduction electrons corresponds to one electron per atom.

The plots of $\bar{m}_{\mathrm{Fe}}(c)$ with allowance for the expression (4.6) at different fixed values of V are shown solid in Fig. 2. Compared with the curve corresponding to a constant value of ϵ_F these curves show a steeper dependence on the iron concentration near certain critical values c_{cr}. At lower values of c the curves shown solid in Fig. 2 are more gently sloping than the dashed curve. These features of the curves of Fig. 2, with the $\epsilon_F(c)$ dependence taken into account, lead to a better agreement between the calculated values of $\bar{m}_{\mathrm{Fe}}(c)$ with the experimental data[5, 9, 10, 16] for the alloys FeNi, FePd, and FePt with fcc lattice.

CONCLUSION

The model assumed in the present paper makes it possible to interpret the main experimental facts on the atomic magnetic moments of iron in d-metals. One such fact is the considerable difference between the atomic magnetic moments of the γ and α modifications of iron. The solid curve in Fig. 1 shows that at a certain V the value of m_{Fe} of γ-Fe decreases steeply to zero. However, according to the experimental results[1, 2] this iron modification has a small atomic moment. The fact that γ-Fe has a small m_{Fe} is probably due to the so-called antiferromagnetism of the collectivized electrons. This phenomenon is the result of the interaction between electrons, which has a collective character and is not accounted for by the Hamiltonian (1.1).

The employed model provides a simple explanation of the experimental results of[3-10, 16], which show that the impurity iron atoms in d-metals with fcc lattice have relative large and approximately equal magnetic moments. In addition it is possible to interpret the behavior of the localized magnetic moments of iron in its alloys with some of these d-metals.

Experiments[5, 9, 10, 16] show that the magnetic moments of the iron atoms in FeNi, FePd, and FePt alloys with fcc lattice remain practically constant when the iron concentration is increased to 60–70 at.%. At a higher iron concentration, the spontaneous magnetization decreases abruptly. These properties indicate that there exist for these alloys critical numbers N_{cr} of the iron atoms surrounding the central atom. If the number of surrounding iron atoms exceeds N_{cr}, then m_{Fe} of the central atom vanishes jumpwise. This conclusion concerning the behavior of m_{Fe} in the indicated alloys was drawn earlier in.[19, 20] It is confirmed by the experimental results on the properties of the iron clusters produced in CuFe alloys.[21, 22] In the present paper, the fact that m_{Fe} remains approximately constant when the number of the surrounding iron atoms increases to N_{cr} is connected with the transitions of the s electrons to d levels. This follows from the shapes of the curves of Fig. 2.

The rapid decrease of the spontaneous magnetization with increasing iron concentration in γ-FeNi, γ-FePd, and γ-FePt alloys is closely connected with their invar anomalies. The physical singularities of the invar alloys are the result of instability of their spontaneous magnetization relative to different external actions (magnetic fields, changes of temperature, and others). This instability of the spontaneous magnetization is due to the fact that the iron concentration in invar alloys corresponds to the steep part of the $\overline{m}_{Fe}(c)$ plot.

Thus, a simple model of localized magnetic moments, which takes interatomic transitions into account, makes it possible to interpret all the main features of the behavior of m_{Fe} in d metals with fcc lattice.

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Translated by J. G. Adashko