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Abstract

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PHYSICS

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MAGNETIC MOMENT AND FIELD AT THE NUCLEUS OF AN ATOM OF A FERROMAGNET

(Presented by Academician N. V. Belov on 6 May 1965)

The aim of the present work is to show that the magnetic moment and the field at the nucleus of an atom are connected with the crystal structure (c.s.) of a ferromagnet and that taking this connection into account makes it possible to explain a number of important phenomena.

The observed distances r_1 between an atom and its nearest neighbors in the c.s. of the transition elements of the iron group (t.e.i.g.) are almost identical, whereas the distance between the $3d$-levels of neighboring Fe, Co, Ni atoms is noticeably larger than for the t.e.i.g. to the left of Fe. As a result, in the first case the $3d$-band is narrower and its overlap with the broad $4s$-conduction band (s–d hybridization) is smaller than in the second. This is partly connected with the absence, in the latter case, of spontaneous spin polarization ([1]).

To explain the phenomena mentioned and others, Friedel compares r_1 with the mean radii of the $3d$-shells of atoms. For the same purpose we introduce a characteristic interatomic distance R:

$$R = 0.13\,[(C/2)^2 - 5.75C + 51] \quad \text{for } C \geqslant 8,$$

$$R = 0.13\,[(C/2)^2 - 4.75C + 43] \quad \text{for } C \leqslant 8, \tag{1}$$

where C is the electron concentration (the sum of the numbers of $3d$- and $4s$-electrons) of the isolated atom.

For a binary disordered ferromagnetic alloy the author introduces the parameters p_a and $\bar{p}$:

$$p_a = 0.64 \sum n_i(r_i - R_a)/\text{Å}, \qquad \bar{p} = 0.64 \sum n_i(r_i - \bar{R})/\text{Å}, \tag{2}$$

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where n_i is the number of neighbors of an atom; $i = 1$ for nearest neighbors; $i = 2$ for next-nearest neighbors; c_a is the atomic concentration of component a of the alloy, $\bar{R} = c_a R_a + c_b R_b$.

It is seen from Table 1 that for nickel $p > 0$, whereas for the other t.e.i.g. $p < 0$. This is one of the examples of the fundamental difference, in Friedel's expression ([2]), among the t.e.i.g.

1. The local atomic magnetic moment m_a, in Bohr magnetons, is calculated according to the relation proposed by us:

$$m_a/\mu_B = \pm \left[M_a + c_k^2 p_a - c_b \bar{p}/e(-1)^e \right], \tag{3}$$

where the upper and lower signs correspond to the alternative A- and B-solutions given by magnetic neutron diffraction for the indicated moment. $M = N_d - 1$ and $M = C - 1$ for "normal" and "anomalous" alloys, respectively.* N_d is the number of unpaired $3d$-electrons of the isolated atom; k and e are given in Tables 2 and 3.

* Normal alloys follow, and anomalous alloys do not follow, the Slater-Pauling curve for magnetization. Friedel ([1]) applies to normal alloys a relation containing a negative number $\bar{Z}$ (the difference of the atomic numbers of components a and b), and to anomalous alloys the number $Z + 10 = C_a$, if b = Ni, and $Z + 10 = C_a + 1$, if b = Co. In both latter cases we take $C_a - 1$.

Table 1

A-moments and the parameter p for pure transition elements of the iron group

	V	Cr	Mn	Fe	Co	Ni	Cu
Transition elements with their own c.c.							
c.c.	b.c.c.	b.c.c.	b.c.c.	b.c.c.	h.c.p.	f.c.c.	f.c.c.
n_1	8	8	8	8	6	12	12
r_1, Å	2.609	2.493	2.494	2.478	2.499	2.487	2.551
n_2	6	6	6	6	6	–	–
r_2, Å	3.011	2.878	2.878	2.861	2.507	–	–
R, Å	3.315	3.055	2.86	2.73	2.535	2.405	2.34
p	−4.78	−3.57	−1.80	−0.79	−0.25	+0.63	+1.62
$N_d - 1$	4	4	4	3	2	1	−1

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Fig. 1

Figure 1: Fig. 1

	V	Cr	Mn	Fe	Co	Ni	Cu
m, μ_B calc.	0.78	0.43	2.20	2.21	1.75	0.63	–
m, μ_B exper.	–	0.40([6])	1.54 ([7])2.50 ([7])	2.22([6])	1.71 ([6])	0.60 ([6])	–
Transition elements with c.c. realized in alloys							
c.c.	f.c.c.	f.c.c.	f.c.c.	f.c.c.	b.c.c.	b.c.c.	b.c.c.
n_1	12	12	12	12	8	8	8
r_1, Å	2.609	2.493	2.494	2.478	2.499	2.487	2.551
n_2	–	–	–	–	6	6	6
r_2, Å	–	–	–	–	2.884	2.870	2.944
p	−5.44	−4.33	−2.82	−1.94	+1.16	+2.21	+3.38

For pure transition elements in (3) the upper sign is taken, $M = N_d - 1$, $c_k = 1$, $c_b = 0$; see Table 1. It is seen from the table that, in the space between neighboring atoms in the c.c. of Fe, Co, and Ni, constant spin moments equal to p, μ_B must be distributed–negative moments in the case of Fe and Co and a positive moment for Ni; this, using the technique of polarized neutrons, has recently been confirmed by Moon ([3]) for Co (h.c.p.).

Fig. 1. Concentration dependence of the moment m_{Fe} of iron in Fe-Ni and Fe-Cr alloys. Solid curves are calculated. Measured values: a–according to data ([10]); b–according to data ([8]); v–according to data ([5]).

In Table 2 and in Fig. 1 the measured and calculated values of the A-moments of Fe in normal Fe-Ni and Fe-Cr alloys, differing in e, are compared. For both alloy systems there is a critical concentration c_{cr}, at which the magnetic moment of metal b (Fe in the first alloy, Cr in the second) changes its orientation to the opposite one; c_{cr} is determined from the condition $a = \bar{R}$, where a is the lattice constant for b.c.c. alloys, and $a = r_1$ for f.c.c. alloys. Such a phenomenon can occur if $R_b > a$ and $R_a < a$. The latter condition is satisfied for Fe–V alloys,

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for which we ([4]) predicted the course of the phenomenon described and, in particular, the magnetic moment of V in Fe, recently confirmed experimentally by Collins and Low ([5]).

Experimental and calculated data for the values of the A- and B-moments of normal and anomalous a(b) are given in Table 3. From the latter it is seen that, in the case of normal alloys, the A-moment $m_{\mathrm{Fe}} < 3\mu_B$, if $b = \mathrm{Ni}$, and $m_{\mathrm{Fe}} > 3\mu_B$, if $b = \mathrm{Co}$, because $p_{\mathrm{Ni}} > 0$, and $p_{\mathrm{Co}} < 0$. For a(b) $\bar{p} = p_b$.

2. The effective magnetic field $H_{\mathrm{eff},a}$ at the nucleus of atom a(b) is calculated from the relation proposed by us:

$$H_{\mathrm{eff},a}/10^2 \text{ kOe} = -\left[M_a + c_k^2 p_a - \beta p_b / e(-1)^e\right], \tag{4}$$

where $\beta = 2$, if $n_1 = n_2$ (h.c.p.); $\beta = 1$, if $n_1 \neq n_2$ (b.c.c. and f.c.c.).

Table 2

***A*-moments of Fe in Fe–Ni and Fe–Cr alloys**

Fe, at. %	n_1	r_1, Å	n_2	r_2, Å	p_{Fe}	$\bar{p}$	m_{Fe}, μB calc.	m_{Fe}, μB exp.
Fe–Ni alloys ($e = 2$, $\kappa = a$)								
91	8	2,479	6	2,861	−0,79	−0,51	2,35	2,41 0,04 ([8])
83	8	2,479	6	2,861	−0,79	−0,28	2,46	2,51 ([9])
76	8	2,479	6	2,861	−0,79	−0,08	2,54	
60	12	2,539	–	–	−1,54	−0,46	2,54	2,44 0,08 ([8])
50	12	2,528	–	–	−1,58	−0,31	2,68	2,60 0,1 ([10])
40	12	2,521	–	–	−1,63	−0,11	2,77	2,72 0,16 ([10])
30	12	2,505	–	–	−1,76	+0,02	2,85	2,66 0,09 ([8])
25	12	2,508	–	–	−1,73	+0,17	2,83	2,91 0,2 ([10])
10	12	2,495	–	–	−1,85	+0,45	2,78	2,58 0,14 ([8])

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Fe, at. %	n_1	r_1, Å	n_2	r_2, Å	p_{Fe}	$\bar{p}$	m_{Fe}, μB calc.	m_{Fe}, μB exp.
0	12	2,487	–	–		+0,63	2,69	2,8 0,2 [5]
Fe–Cr alloys ($e = 1$, $\kappa = a$)								
85	8	2,483	6	2,865	−0,77	−1,19	2,26	2,24 0,10 [10]
71	8	2,464	6	2,867	−0,77	−1,57	2,15	2,13 0,12 [10]
54	8	2,486	6	2,870	−0,74	−1,98	1,88	1,75 0,17 [10]

Table 3

Magnetic moments and fields at the nuclei of atoms of solid solutions $a(b)$

a	M_a	b	c.s.b	p_b	p_a^*	κ	e	m_a, μB calc.	m_a, μB exp.	H_{eff}, kOe calc.	H_{eff}, kOe exp.
***A*-moments and H_{eff} of normal** $a(b)$											
Fe	3	Ni	f.c.c.	+0,63		a	2	2,7	2,8 0,2 [5]	−270	283 [11]
Fe	3	Co	h.c.p.	−0,25		a	2	3,12	3,1 [9]	−325	−329 [11]
Fe	3	Cr	b.c.c.	−3,56		a	1	−0,56		+56	+35 [12]
Fe	3	Cr	b.c.c.	−3,56		a	1	−0,56		+56	+60 [13]

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a	M_a	b	c.s.b	p_b	p_a^*	κ	e	m_a, μB calc.	m_a, μB exp.	H_{eff}, kOe calc.	H_{eff}, kOe exp.
Fe	3	V	b.c.c.	−4,78		a	1	−1,78		+178	+180 [13]
Cr	0	Fe	b.c.c.	−0,79		a	1	−0,8	−1 [10]	+80	<100 [11]
V	0	Fe	b.c.c.	−0,79		a	1	−0,8	−0,8 [5]	+80	90 [11]
Cu	−1	Fe	b.c.c.	−0,79		a	1			−170	−213 [11]
Cu	−1	Co	h.c.p.	−0,25						−150	157 [11]
Cu	−1	Ni	f.c.c.	+0,63						−40	−45 [11]
Co**	2	Fe	b.c.c.	−0,79		a	2		1,6 [15]	−280	−286 [11]
Ni**	1	Fe	b.c.c.	−0,79		a	2		1 [8,10]	−220	235 [11]
Fe^{57}	3	Fe	b.c.c.	−0,79		a	2			−342	−339 [11]
Co^{59}	2	Co	f.c.c.	−0,25		a	2			−212	−215 [11]
Ni^{61}	1	Ni	f.c.c.	+0,63		a	2			−66	75 [11]
Ni	1	Co	h.c.p.	−0,25		b	2			−188	189 [11]
Co**	2	Ni	f.c.c.	+0,63		b	2			−119	−120 [11]
***B*-moments of** $a(b)$											
Ni	1	Fe	b.c.c.	−0,79	+2,21	b	2	3,61	3,5 [8]	−360	360 [13]
Co	2	Fe	b.c.c.	−0,79	+1,16	b	2	3,56		−356	360 [13]
Fe	3	Ni	f.c.c.	+0,63	−1,94	b	1	−1,7	−1,7 [10]		
Cr	−1	Fe	b.c.c.	−0,79	−3,56	b	1	+5,35	+5,4 [10]		
V***	−0,8	Fe	b.c.c.	−0,79	−4,78	b	1	+6,37			
Cr	+1	Co	h.c.p.	−0,25	−4,33	b	2	+3,1	+3 [10]		

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a	M_a	b	c.s.b	p_b	p_a^*	κ	e	m_a, μB calc.	m_a, μB exp.	H_{eff}, kOe calc.	H_{eff}, kOe exp.
A-moments and H_{eff} of anomalous $a(b)$											
Cr	5	Co	h.c.p.	−0,25	−4,33	b	2	0,92	+1 [10]		
Cr	5	Ni	f.c.c.	+0,63	−4,33	b	2	0,35	+0,6 [5]	1,0	
V	4	Ni	f.c.c.	+0,63	−5,44	b	1	−0,81	−1,2 [5]	0,4	
Mn	6	Ni	f.c.c.	+0,63	−2,82	b	2	2,81	2,4 [5]	−287	−316 [11]
Mn	6	Ni	f.c.c.	+0,63	−2,82	b	2	2,81	2,4 [5]	−287	−325 [11]
Mn	6	Co	h.c.p.	−0,25	−2,82	b	1			−270	200 [11]
V	4	Co	h.c.p.	−0,25	−5,44	b	1			−194	183 [11]
Fe	7	Ni	f.c.c.	+0,63	−1,94	b	2			−475	470 [13]
Fe	7	Co	h.c.p.	−0,25	−1,94	b	2			−531	520 [13]

* The values of p_a are the same as they would be if the dissolved a had the coordination number of the matrix b.

** Before the third term in (4) the factor $1 - z$ is taken, where z is the negative difference C_a and C_b.

*** Reduced to the observed values of the A-moments $a(b)$ for M_a.

From Table 3 and Figs. 2 and 3 it is seen that at the nucleus of an iron atom in nickel $H_{\text{eff}} < 300$ kOe, while in cobalt $H_{\text{eff}} > 300$ kOe (for the reason indicated above). Extrapolation of the rectilinear portions of the curves in Figs. 2 and 3 to 100 at.% Fe gives $H_{\text{eff}} = 360$ kOe, which is close to the calculated value of H_{eff} at

Fig. 2

Fig. 3

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Fig. 2

Figure 2: Fig. 2

Fig. 3

Figure 3: Fig. 3

the nuclei of Co and Ni atoms dissolved in Fe (Table 3). An analogous extrapolation to 100 at.% Co gives $H_{\text{eff}} = 520$ kOe, and to 100 at.% Ni (Fig. 2) gives $H_{\text{eff}} = 470$ kOe at the Fe nucleus (see Table 3).

The measured values of $H_{\text{eff},a}/10^2$ kOe at the nuclei of Sn^{119} dissolved in Fe, Co, and Ni agree in sign with the parameter p_b for the indicated matrices (4). The quantities compared are almost equal in absolute value (see Table 4).

Table 4

H_{eff} at Sn^{119} nuclei in Fe, Co, Ni

Nucleus a	Matrix b	$H_{\text{eff}}/10^2$ kOe, exp. (16)	p_b
Sn^{119}	Fe	-0.88	-0.79
Sn^{119}	Co	-0.265 ± 0.15	-0.25
Sn^{119}	Ni	$+0.165 \mp 0.01$	$+0.63^*$

* The somewhat larger discrepancy between the compared quantities for Ni is explained by the fact that, in the opinion of the authors of the experiment, the screening of the moment by the valence electrons of tin is greater in this case than for Fe and Co.

For gold dissolved in the same matrices, H_{eff} has discrete values (4); for example, for gold in iron

$$H_{\text{eff}}/10^2 \text{ kOe} = -\alpha(C_b - 1)p_b,$$

where $\alpha = 1, 2, 3$, and 4.

3. The coefficient 0.64 in (2) is $\chi/2 \cdot 10^2$ kOe, where χ is the observed value of the hyperfine-structure interaction parameter for divalent ions of transition elements. In this case

$$\sum n_i(r_i - R)/2\text{Å}$$

gives the number $n_{3d(4s)}$ of unpaired $3d$-electrons in the $4s$-conduction band; the number n_{4s} of unpaired $4s$-electrons in it is equal to $p - n_{3d(4s)}$. For Fe the first number is -0.61 ($m_d = 2.39$), and the second is -0.18 (the experiment of Shull and Yamada gives 2.39 and -0.21); for Co (hcp)

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-0.19 ($m_d = 1.81$) and -0.06 (Moon' s experiment gives 1.86); for Ni 0.49 ($m_d = 1.51$) and 0.1 ($-1 + 0.1 = -0.9$).

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