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Abstract

Full Text

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EFFECTIVE MAGNETIC FIELDS AT ATOMIC NUCLEI OF FERROMAGNETS

(Presented by Academician N. V. Belov, October 7, 1964)

It is known that large effective magnetic fields H_{eff} act on the atomic nuclei of ferromagnets and that the latter are usually negative, i.e., antiparallel to the direction of the magnetization vector. In paper (^{1}) it is indicated that comparison with experimental data reveals the weakness of the theory, and therefore at present it is expedient to seek empirical relations for calculating H_{eff}. Such relations are proposed by us below.

First let us consider the pure metals Fe, Co, Ni. The first of the indicated relations has the form

$$H_{\text{eff}} = -[10^2 m/\mu_B - H_s]\ \text{kOe}, \tag{1}$$

where m is the atomic magnetic moment, μ_B is the Bohr magneton, $H_s = N_s(\downarrow)H_A(\downarrow)$. Here $N_s(\downarrow)$ is the number of unpaired (with spins antiparallel to the spin of the 3d-shell) conduction electrons in the 4s-band of the metal, $H_A(\downarrow)$ is the negative contribution to H_{eff} of a 4s-electron (with spin antiparallel to the spin of the 3d-shell) of an isolated atom, calculated in paper (^{2}) by the Hartree-Fock method. The first and second terms of (1) give the contributions due to the Fermi contact interaction of the nucleus, respectively, with the inner s-electrons of the ionic cores of the crystal lattice and with the outer 4s-conduction electrons polarized by the unpaired 3d-electrons of the same cores.* In order to measure directly the contribution H_s, in paper (^{3}) the Mössbauer effect was studied on ^{119}Sn nuclei dissolved in Fe, Co, and Ni. The values of $H_s/10^5$ Oe thereby obtained are close to the values of the quantity p introduced by us (^{4}), related to the contribution to the moment m of conduction electrons (see Table 1).

Fig. 1. Concentration dependence of H_{eff} at ^{57}Fe nuclei in Fe—Ni alloys. *a* —experimental data; *b* and *c* —calculated: *b* —data for m from work (12) were used, *c* —from work (13).

Let us find $N_s = H_s/H_A$ from the experimental data (3). The numbers thus obtained are close to $N_s = 0.1|p|$; the latter expression is used by us in calculating the second term for Fe, Co, Ni, and for alloys. The second of the indicated relations has the form:

$$H_{\text{eff}} = -(m/\mu_B - 1.5p) \cdot 10^2 \text{ koersted}, \tag{2}$$

Table 1

Magnetic fields at the atomic nuclei of tin and ferromagnetic metals

Metal (structure)	p, calc. (4)	$H_s/10^5$ oersted, expt. (3)	$H_A(4s\downarrow)$, koersted *, calc. (2)	N_s, expt. (3)	N_s, calc. (4)	m, μ_B, expt.	H_{eff}, koersted, calc. from (1)	H_{eff}, koersted, calc. from (2)	H_{eff}, koersted, expt.
Fe (bcc)	−0.80	−0.88	−1361	0.065	0.080	2.22	−331	−342	−342 (11)
Co (hcp)	−0.26	−0.26	−1574	0.017	0.026	1.74	−215	−213	−215 (11)
Co (fcc)	−0.40	–	−1574	–	0.040	1.71	−234	−231	−228 (2)
Ni (fcc)	−0.20	+0.16	−1800	0.008	0.020	0.60	−96	−90	−90 (20), −60 (11)

* $H_A(4s\uparrow) = +1850,\ +1951$ and $+2053$ koersted for Fe, Co, and Ni, respectively (↑—spin parallel to the spin of the $3d$ shell; ↓—spin antiparallel).

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* In paper (2) it is assumed that the first contribution is equal to $-126(m/\mu_B)$ kOe and that, in agreement with Marshall (5), $H_s > 0$; therefore in paper (2) (in it $H_s = N_s(\uparrow)H_A(\uparrow)$ for Fe) $H_A > 0$ is used. In all cases considered below, however, we use $H_A < 0$, since, as experiment shows (3,6,7), $H_s < 0$. Marshall, who earlier had supposed that $H_s > 0$, taking into account the results of studies (8,9) showing that the contributions of conduction electrons to m and to H_{eff} are negative, acknowledges in paper (10) that $H_s < 0$.

Fig. 2. Dependence of the fields H_s at the nuclei of diamagnetic elements (^{198}Au, ^{199}Au, ^{119}Sn, etc.) dissolved in Fe, Co, Ni on the number N_s of unpaired conduction electrons in the 4*s* band of the solvents. The straight lines were calculated (present work). Points are experimental data: *a*—from (^{15}); *b*—(^{6}); *v*—(^{17}); *g*—(^{7}); *d*—(^{16}); *e*—(^{18}); *zh*—(^{19}); *z*—(^{3}).

Figure 2: Fig. 2. Dependence of the fields H_s at the nuclei of diamagnetic elements (^{198}Au, ^{199}Au, ^{119}Sn, etc.) dissolved in Fe, Co, Ni on the number N_s of unpaired conduction electrons in the 4*s* band of the solvents. The straight lines were calculated (present work). Points are experimental data: *a*—from (^{15}); *b*—(^{6}); *v*—(^{17}); *g*—(^{7}); *d*—(^{16}); *e*—(^{18}); *zh*—(^{19}); *z*—(^{3}).

$H_s/p = 150$ (koersted); the same value is possessed by H_{eff}/m for the pure ion (^{1}). Tables 1 and 2 and Fig. 1 compare the values of H_{eff} calculated from (1)–(2) with the experimental values.

We shall now find N_s from the data of works ($^{6-7,\ 15-18}$). It is seen from Table 3 that, for solutions of gold in iron, the measured values of H_s are in approximately the ratios $1:2:3:4$, while the values of N_s found are close to the following discrete numbers: $0.5|p| = 0.4$; 0.8; 1.2 and 1.6, i.e., 5, 10, 15, and 20 times larger than in the case of pure iron ($0.1|p| = 0.08$). The calculated values of H_s corresponding to these discrete N_s values are also discrete, and the measured values of H_s are grouped around them; fields at the nuclei of impurity atoms have not yet been found for intermediate values of N_s.

Analogous regularities are observed upon dissolving gold in Co and Ni (see Table 3 and Fig. 2).

Fig. 2. Dependence of the fields H_s at the nuclei of diamagnetic elements (^{198}Au, ^{199}Au, ^{119}Sn, etc.) dissolved in Fe, Co, Ni on the number N_s of unpaired conduction electrons in the 4*s* band of the solvents. The straight lines were calculated (present work). Points are experimental data: *a*—from (^{15}); *b*—(^{6}); *v*—(^{17}); *g*—(^{7}); *d*—(^{16}); *e*—(^{18}); *zh*—(^{19}); *z*—(^{3}).

Thus, the fields considered at the nuclei of diamagnetic elements dissolved in Fe, Co, Ni apparently depend mainly on the solvent metal (in particular, on the quantity *p* characterizing it). The fact described recalls the appearance and disappearance of "giant" localized magnetic moments in dilute solid solutions of iron in nonmagnetic elements, observed at quite definite electron concentrations (^{9}).

Table 2

Magnetic fields at ^{57}Fe nuclei in ferromagnetic alloys

Alloy (metal)	Fe, at. %	n_1	r_1, Å	n_2	r_2, Å	p	m, μ_B	H_{eff}, kOe, calc. by (1)	H_{eff}, kOe, calc. by (2)	H_{eff}, kOe, exp.
Fe *	100	8	2,478	6	2,861	−0,80	2,22	−331	−342	−342 (14)
Fe – Co *	50	8	2,475	6	2,847	−0,22	3,15 (12)	−345	−348	−345 (14)
Fe – Co *	35	8	2,466	6	2,836	−0,12	3,15 (12)	−331	−333	−336 (14)
Fe – Co *	27	8	2,456	6	2,825	−0,07	3,15 (12)	−324	−325	−333 (14)
Fe – Ni *	91	8	2,479	6	2,861	−0,66	2,40 (12)	−330	−339	−342 (14)
Fe – Ni **	60	12	2,529		–	−0,52	2,44 (12)	−320	−322	−315 (14)
Fe – Ni **	50	12	2,528		–	−0,40	2,60 (13)	−314	−320	−306 (14)
Fe – Ni **	40	12	2,521		–	−0,28	2,71 (13)	−300	−313	−309 (14)
Fe – Ni **	26	12	2,508		–	−0,11	2,91 (13)	−300	−307	−291 (14)
Fe – Cr *	85	8	2,483	6	2,865	−0,56	2,24 (13)	−300	−308	−292 (14)

Alloy (metal)	Fe, at. %	n_1	r_1, Å	n_2	r_2, Å	p	m, μ_B	H_{eff}, kOe, calc. by (1)	H_{eff}, kOe, calc. by (2)	H_{eff}, kOe, exp.
Fe–Cr *	71	8	2,484	6	2,867	−0,38	2,13 (13)	−265	−270	−255 (14)
Fe–Cr *	54	8	2,486	6	2,869	−0,19	1,75 (13)	−201	−203	−206 (14)
Fe–V *	84	8	2,484	6	2,864	−0,54	2,21 (4)	−294	−302	−298 (14)
Fe–V *	71	8	2,489	6	2,872	−0,35	1,92 (4)	−240	−246	−244 (14)
Fe–V *	61	8	2,502	6	2,887	−0,21	1,74 (4)	−203	−205	−205 (14)
Fe–V *	51	8	2,525	6	2,914	−0,11	1,41 (4)	−156	−157	−162 (14)
Fe–Al *	75	8	2,50		–	−0,66	2,16 (14)	−306	−316	−295 (14)
Fe–Al *	75	4	2,50		–	−0,33	1,46 (14)	−191	−196	−212 (14)
Fe in Co *	0					0	3,15 (12)	−315	−315	−315 (14)
Fe in Ni *	0					0	2,80 (12)	−280	−280	−280 (14)
Co in Fe *	100					−0,80	2,00 (12)	−309	−320	−320 (2)

Alloy (metal)	Fe, at. %	n_1	r_1, Å	n_2	r_2, Å	p	m, μ_B	H_{eff}, kOe, calc. by (1)	H_{eff}, kOe, calc. by (2)	H_{eff}, kOe, exp.
Ni in Fe *	100					$-0,80$	1,00 (12)	−209	−220	−195 (11)

Note. $p = [0,63\lambda^2 \sum n_i(r_i - R)/A + \beta]/(1-\beta)$, where r_i and n_i are, respectively, the interatomic distance and the number of nearest-neighbor atoms in the coordination sphere of the lattice; λ is the atomic concentration of Fe; $R = 0,13[(3,75 - C/2)^2 + K(8-C)^2 + 21]$; here C is the electron concentration (the number of $3d$- and $4s$-electrons) of the isolated atom; $K = 2$ for $C > 8$; $K = 1$ for $C \leq 7$; $\beta = -1$ for pure Ni; $\beta = 0$ for Fe and Co. The values of the two arbitrary constants, K and β, are given, each of them taking only two values (2 or 1 for K and −1 or 0 for β). For all cases given in Table 2, $R = 2,733$ Å and $H_A = -1361$ kOe. In 18 cases the alloys have a b.c.c. structure (*), and therefore for them all quantities (except λ) entering the second term of (1) are the same; with constant m, the field H_{eff} should vary parabolically (as the square of the concentration λ), which is indeed observed experimentally; see Fig. 1. In 4 cases the alloys have an f.c.c. structure (**).

Table 3

Magnetic fields at the nuclei of atoms of diamagnetic elements in Fe, Co, Ni

Nucleus	Solvent	p	N_s	$N_s/\lvert p \rvert$	H_A, kOe	H_s, kOe, calc. by (1)	H_s, kOe, exp.
^{57}Fe	Fe (b.c.c.)	$-0,8$	0,08	0,1	−1361	−109	
^{198}Au	Fe (b.c.c.)	$-0,8$	0,40	0,5	−1361	−544	500–700 (15)
^{198}Au	Fe (b.c.c.)	$-0,8$	0,80	1	−1361	−1090	−1000 (6)
^{198}Au	Fe (b.c.c.)	$-0,8$	1,20	1,5	−1361	−1633	1600 (16)
^{197}Au	Fe (b.c.c.)	$-0,8$	1,20	1,5	−1361	−1633	−1420(7), 1460(17)
^{199}Au	Fe (b.c.c.)	$-0,8$	1,60	2	−1361	−2178	> 2000 (18)

Nucleus	Solvent	p	N_s	$N_s/\lvert p\rvert$	H_A, kOe	H_s, kOe, calc. by (1)	H_s, kOe, exp.
^{63}Cu	Fe (b.c.c.)	$-0,8$	0,16	0,5	-1361	-218	213 (15)
^{122}Sb	Fe (b.c.c.)	$-0,8$	0,16	0,2	-1361	-218	200 (15)
^{141}In	Fe (b.c.c.)	$-0,8$	0,16	0,2	-1361	-218	180 (15)
^{61}Ni	Ni (f.c.c.)	$-0,2$	0,02	0,1	-1800	-36	
^{198}Au	Ni (f.c.c.)	$-0,2$	0,1	0,5	-1800	-180	-180 (6)
^{197}Au	Ni (f.c.c.)	$-0,2$	0,2	1	-1800	-360	-340(7), 420(17)
^{59}Co	Co (h.c.p.)	$-0,4$	0,04	0,1	-1574	-63	
^{197}Au	Co (h.c.p.)	$-0,4$	0,6	1,5	-1574	-944	-980(7), -990(7)
^{197}Au	Co (h.c.p.)	$-0,4$	0,8	2	-1574	-1260	1180 (17)
^{63}Cu	Co (h.c.p.)	$-0,4$	0,1	0,25	-1574	-157	157 (19)
^{119}Sn	Fe	$-0,8$	0,08		-1361	-109	-88 (3)
^{119}Sn	Co	$-0,26$	0,026		-1574	-41	-26 (3)
^{119}Sn	Ni	$-0,2$	0,01		-1800	-18	$+16$ (3)

In the case of Fe and Co ($r_1 < R$), the conduction electrons are also in the $3d$ band (s–d hybridization) and give a positive contribution, which is compensated ($\beta = 0$) by the negative contribution due to antiferromagnetic polarization (2,9). In the case of Ni this hybridization is absent (because $r_1 > R$), and there is only the above-mentioned negative contribution ($\beta = -1$), which reduces both H_{eff} by 10^3 oersted ($H_{\text{eff}} = -190$ instead of -90 oersted, according to (1)–(2)), and the moment $m = (N_d - 1 + 0.63 \sum n_i(r_i - R)/\text{Å})\mu_B$ by $\beta\mu_B$ (0.6 instead of 1.6 μ_B at $\beta = 0$). N_d is the number of unpaired $3d$-electrons of the isolated atom. Compression of Ni, under which it turns out that $r_1 \leqslant R$ ($\beta = 0$), should lead to a moment of $1\mu_B$ (instead of the $0.6\mu_B$ observed experimentally).

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