Hyperfine interactions and local magnetic moments in the intermetallic compound $ZrFe_2$ containing 3*d*-element impurities

V. S. Pokatilov

Central Research Institute for Ferrous Metallurgy

(Submitted 21 November 1986)
Zh. Eksp. Teor. Fiz. **93**, 944–951 (September 1987)

The hyperfine fields at ^{91}Zr nuclei in the compound $ZrFe_2$ containing 3*d*-atom impurities were measured. The local magnetic moments μ_Z of the 3*d* atoms are estimated. The dependence of μ_Z on the atomic number Z of the atom in the periodic table is oscillatory with a maximum $\mu_Z = +3.05\mu_B$ for $Z = 25$ (Mn) and a minimum $\mu_Z = -0.85\mu_B$ for $Z = 23$ (V). The sign of μ_Z is reversed at $Z = 23$–24. The contribution to the hyperfine field H_0 at ^{91}Zr nuclei in $ZrFe_2$ from the first coordination sphere (of the iron atoms) estimated at $H^{(1)} = -237$ kOe. The constant of polarization of the *s* electrons by the magnetic moments of the iron atoms is $A_1 = -125\ \mathrm{kOe}/\mu_B$. The magnetic moment at the zirconium atoms is estimated from data on the hyperfine fields to be $\mu_{Zr} = -(0.5 \pm 0.1)\mu_B$.

INTRODUCTION

It was shown theoretically[1,2] and experimentally[3] that the magnetic moments μ_Z at transition-atom impurities in an iron matrix differ in magnitude and in sign, depending on their place in the series of the 3*d* elements, and that this variation is oscillatory (*s*-shaped). According to Ref. 1 this is due to peculiarities of the electronic structure of the impurity atoms in the iron matrix.

It was of interest to determine the strengths of the hyperfine fields (HFF) and of the local magnetic moments, as well as to investigate the character of their distributions for different *s*-, *p*-, and *d*-elements in matrices of other transition metals, alloys, or compounds, for in this case the differences between the electronic structure of the alloy or compound from that of pure iron can introduce singularities both in the values of the HFF or of the magnetic moments at the impurity atoms, and in the character of their distribution. Such investigations are important for the understanding of the nature of hyperfine interactions and of the magnetic moments at transition-element atoms in various alloys, for the theory of their alloying and for their practical applications.

Pulsed nuclear magnetic resonance (NMR) was used in the present study to measure the HFF at ^{91}Zr nuclei and of some impurity atoms of 3*d* elements, and to estimate the magnetic moments at 3*d*-element atoms located in a matrix of the Laves-type compound $ZrFe_2$. The $ZrFe_2$ compound has a cubic structure of the $MgCu_2$ type, and is a ferromagnet with a Curie temperature $T_C = 630$ K. It was usually assumed that only the iron atoms of this compound have magnetic moments. Recent[4,5] calculations of the electronic structure of $ZrFe_2$ as well as data on the pressure dependence of the HFF and of the magnetic moment of the alloy have shown that, besides the iron atom, the zirconium atom also has a magnetic moment. We present here additional proof of the existence of magnetic moment at the zirconium atoms in $ZrFe_2$ and consider the nature of the HFF at the ^{91}Zr nuclei in Laves alloys based on iron.

SAMPLES AND MEASUREMENT PROCEDURES

A set of alloys $ZrFe_{2-x}B_x$ and $Zr_{1-y}C_yFe_2$, was smelted, where B stands for Al, Ti, V, Cr, Mn, Co, Ni and Cu and C for Sc and Cu. The impurity-atom content was $x = 0.02$ (1.3 at.%) and 0.05 (3.3 at.%), and $y = 0.01$, 0.02 and 0.05 (0.03, 0.66 and 1.65 at. %, respectively). The alloys were smelted in an arc furnace out of stoichiometric mixtures of highly purified metals. The billets were ground up and remelted. This operation was repeated several times. The samples were cooled from the liquid state to room temperature on the copper table of the furnace. The investigated samples (powders of size $\leqslant 70\ \mu$m) were made both out of billets subjected to homogenization and from billets cooled in the furnace. It turned out that annealing had practically no effect on the measured parameters. An x-ray diffraction analysis of the powders has shown that the samples were single-phase and had an $MgCu_2$ structure. NMR was used to measure the HFF at the ^{91}Zr and at several impurity atoms. The NMR spectra were measured point-by-point in the frequency range 20–150 MHz at 4.2 K. The dependence of the echo-signal amplitude on the frequency f was assumed in the form $A_{\text{echo}} \propto f^2$. The NMR spectra of the ^{57}Fe nuclei in the frequency region 25–32 MHz are not reported because no influence of the impurity atoms on the ^{57}Fe atom could be observed in view of the weak signal of these ^{57}Fe nuclei in samples with natural isotope mixture.

The location of the impurities in the $ZrFe_2$ lattice was determined from structural investigations of Laves phases based on iron,[6] from the data on Ref. 7, and also from the NMR results of the present paper on the positions of the satellite peaks on the ^{91}Zr nuclei, whose atoms contain impurity atoms in the nearest spheres.

EXPERIMENTAL RESULTS

Figure 1 shows the NMR spectra of $ZrFe_2$ alloys containing Al and 3*d*-atom impurities. The NMR spectrum of the compound $ZrFe_2$ consists of two groups of resonance lines in the regions 25–32 and 45–60 MHz. The first group pertains to the resonance of the ^{57}Fe nuclei and the second to ^{91}Zr. The NMR spectrum of ^{57}Fe contains two lines, in accord with the two magnetically nonequivalent states of the iron atoms in the $MgCu_2$ lattice. The NMR spectrum of ^{91}Zr has one intense line at ~50 MHz and an unresolved satellite line at ~48 MHz, the nature of which had not been discussed in the literature. The resonance of the ^{91}Zr nuclei at 48 and 50 MHz in $ZrFe_2$ with impurities of other elements is

0038-5646/87/090531-05$04.00

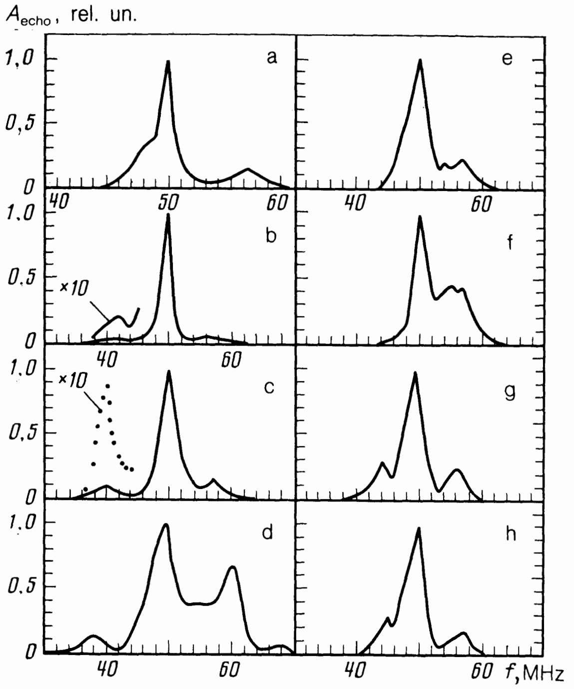

FIG. 1. NMR spectra in the alloys $ZrFe_2$ (a), $ZrFe_{1.98}Al_{0.02}$ (b) $ZrFe_{1.95}Ti_{0.05}$ (c), $ZrFe_{1.95}V_{0.05}$ (d), $ZrFe_{1.95}Cr_{0.02}$ (e), $ZrFe_{1.95}Mn_{0.05}$ (f), $ZrFe_{1.95}Co_{0.05}$ (g), $ZrFe_{1.95}Ni_{0.05}$ (h)

due to the nonequivalence of the directions of the magnetic moments of the zirconium atoms relative to the easy magnetization axes ⟨111⟩, in analogy with what is observed for iron atoms. The magnetic moments at the zirconium atoms also produce dipole fields at the ^{91}Zr nuclei. As seen from Fig. 1, the impurity atoms either enhance or suppress the ^{91}Zr resonance at 48 MHz, i.e., they influence the distribution of the easy-magnetization axes in $ZrFe_2$. In this compound, the zirconium atoms contain 12Fe in the first coordination sphere (CS) and 4Zr in the second CS, while the iron atoms have 6Fe in the first CS and 6Zr in the second CS. The peak at ~57 MHz is due to resonance of ^{91}Zr whose atoms probably contain in the second CS iron atoms in zirconium sites.[8,9] We consider hereafter only the atoms that occupy regular positions in the ordered $ZrFe_2$ lattice.

Introduction of aluminum impurity atoms, which have no magnetic moment, into the iron-atom sites leads to the appearance of additional lines in the spectrum of $ZrFe_{1.98}Al_{0.02}$: 1) a resolved line at 27.5 MHz, due to the ^{27}Al nuclei whose atoms contain 6Fe in the first CS and 6Zr in the second; 2) the peak at ~42 MHz in the ^{91}Zr spectrum, pertaining to the resonance of ^{91}Zr nuclei whose atoms have 11Fe + 1Al in the first CS. The HFF at the ^{27}Al nuclei is equal to − 27.2 kOe (with allowance for the Lorentz field, equal to − 2.4 kOe for $ZrFe_2$). This Lorentz field is taken into account in all the HFF reported hereafter. The nature of the HFF at ^{27}Al nuclei in Laves phases based on iron will be considered later.

It can be seen from the spectra of ZrF_2 alloys containing Ti, V, Cr, Mn, Co, and Ni impurity atoms (see Fig. 1) that the position of the ^{91}Zr satellite lines in the frequency range 38–45 MHz depends on the element introduced into the alloy. Impurity atoms of the 3*d* elements Ti, V, Cr, Mn, Co and Ni occupy the sites of iron atoms in the $ZrFe_2$ lattice and shift the resonance line of the ^{91}Zr nuclei whose atoms contain one impurity atom in the first CS. The HFF shift depends on the atomic number *Z* of the element in the periodic table. The HFF of the satellites for the ^{91}Zr nuclei are given in Table I. The HFF of ^{91}Zr atoms whose nuclei contain impurities in the first CS lie above and below the ^{91}Zr HFF due to the aluminum impurities that have no magnetic moment. This shows that impurity atoms of 3*d*-elements that occupy the sites of the iron atoms in the $ZrFe_2$ lattice have negative or positive magnetic moments relative to the moments of the iron atoms in $ZrFe_2$.

Introduction of chromium and manganese atoms in $ZrFe_2$ leads to the appearance of resonance lines of the ^{91}Zr nuclei on the high-frequency side of the principal line. This indicates that the magnetic moments at these atoms are larger than the magnetic moment $\mu_{Fe} = 1.90\mu_B$ of the iron atoms.[4] Addition of more than 3–4 at. % chromium broadens greatly the principal line, probably because of the stronger chemical interaction between the zirconium and chromium atoms and because of atomic clustering effects.

Vanadium occupies sites of iron atoms in the $ZrFe_2$ compound. The NMR spectrum of the $ZrFe_{1.95}V_{0.05}$ alloy contains, besides the indicated lines in the 348–57 MHz region, an additional line at 60.5 MHz, due to resonance of the ^{51}V nuclei, since the shift of this line in an external magnetic field towards lower frequencies proceeds at a rate determined by the gyromagnetic ratio of the ^{51}V nuclei. Thus, the HFF at the ^{51}V nuclei in the $ZrFe_{1.95}V_{0.05}$ alloy is equal to − 56.3 kOe. An increase (up to 0.10) or decrease (< 0.05) of the vanadium content in the alloy does not change the position of the 60.5 MHz resonance line.

Investigations[10] have shown that scandium atoms occupy sites of zirconium atoms in the $ZrFe_2$ lattice. The NMR spectra of an alloy containing scandium in the form of impurity atoms are shown in Fig. 2. It can be seen from the NMR spectrum of the $Zr_{0.99}Sc_{0.01}Fe_2$ alloy that, besides the ^{91}Zr resonance lines, there appeared additional lines at 63 and 69

TABLE I.

Z	$-H_0$, kOe	$-H_0^{(1)}$, kOe	μ_Z, μ_B	$\mu_{Z'}$, μ_B	Z	$-H_0$, kOe	$-H_0^{(1)}$ kOe	μ_Z, μ_B	$\mu_{Z'}$, μ_B
Al	128.3	108.1	0	0	Mn	128.3	140.6	+3.05	+2.58
Ti	128.3	102.8	−0.48	−0.30	Fe	128.3	128.3	+1.90	+1.72
V	128.0	99.3	−0.84	−0.67	Co	126.7	113.1	+0.48	+0.36
Cr	128.3	139.6	+2.97	+2.02	Ni	128.3	114.1	+0.59	+0.01

Note: The hyperfine fileds at the ^{91}Zr nuclei, whose atoms contain in the first coordination sphere 12Fe (H_0) and 11Fe + 1Z (Z is an impurity atom) (H_0($^{1)}$; μ_Z is the magnetic moment at the impurity atom *Z*, estimated from Eq (3); μ'_Z is the same according to published data.

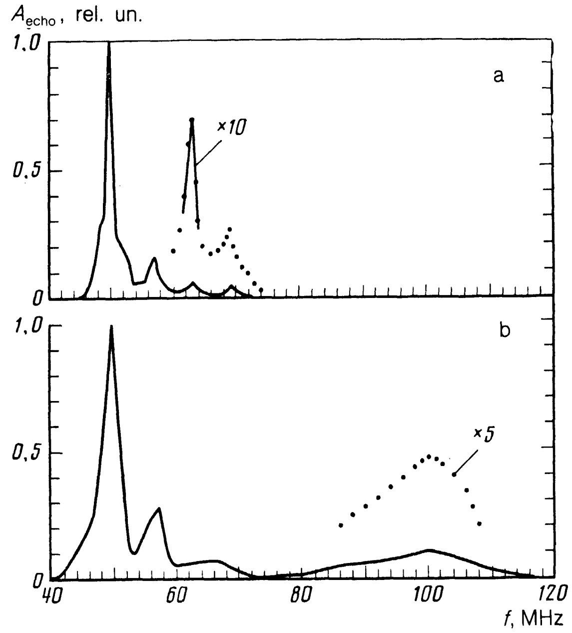

FIG. 2. NMR spectra in the alloys $Zr_{1.99}Sc_{0.01}Fe_2$ (a), $Zr_{0.95}Cu_{0.05}Fe_2$ (b)

MHz, due to the resonance of the ^{45}Sc nuclei, and also an unresolved line at 52.4 MHz. An increase of the scandium content in the alloy resolved the 52.4 MHz line, and the intensity of the peaks at 63 and 69 MHz increased. The line 52.4 MHz pertains to the resonance of the ^{91}Zr nuclei, whose atoms contain a scandium atom in the second CS. The HFF at the ^{45}Sc nuclei in the $ScFe_2$ alloy with $MgCu_2$ structure were measured in Refs. 10–12, and a value $H_0 = -102.5$ kOe (104 MHz) was obtained. The scandium atoms occupy zirconium-atom sites in ZrFe. Assuming that the scandium is randomly distributed over the zirconium sites in the $Zr_{1-y}Sc_yFe_2$ alloy lattice at $y = 0.001$, 0.02, and 0.05 (the NMR sectra of alloys with $y > 0.01$ are not cited here and are discussed in part in Ref. 10), we have estimated the NMR line intensities for ^{45}Sc, whose atoms have 4Zr, 3Zr + 1Sc, etc., in the second Cs. The most probable for these concentrations are configurations with 4Zr. Comparison of the areas of the NMR spectrum peaks of ^{45}Sc alloys with $y = 0.01$, 0.02, and 0.05 with the calculated intensities shows that the resonance of the ^{45}Sc nuclei whose atoms have 4Zr in the second CS are located at 63 MHz. Thus, for the impurity state of scandium in a $ZrFe_2$ matrix, the HFF of the ^{45}Sc nuclei is equal to -63.3 kOe and is smaller by almost 1.8 times than in $ScFe_2$ (Refs. 9 and 10). This is an unexpected result, if it is recognized that the magnetic moment of the iron atoms is smaller in $ScFe_2$ than in $ZrFe_2$.

The NMR spectrum of the $Zr_{0.95}Cu_{0.05}Fe_2$ alloy (see Fig. 2) is similar to that of $ZrFe_{1.95}Cu_{0.05}$ (the latter spectrum is not given here). In addition to the resonance lines of the ^{91}Zr nuclei there is observed a broad peak in the 80–120 MHz region with a maximum at ~100 MHz. This peak pertains to the resonance of the ^{65}Cu nuclei, which have an HFF $|H_0| = 83 \pm 3$ kOe. The sign of the field has not been determined. No resolved satellite peaks were observed in the frequency regions 40–45 and ~52 MHz for an alloy of $ZrFe_2$ with copper. The increased (compared with the statistical value) intensity of the ^{91}Zr spectrum at 40–45 MHz shows that the copper atoms probably occupy iron sites and tend to form clusters with zirconium.

DISCUSSION OF EXPERIMENTAL DATA

The HFF H_0 of a zirconium atom having a magnetic moment and located in a feromagnetic metal matrix will be defined as[13]

$$H_0=H_{cp}+H_s+H_{sp}, \quad (1)$$

where H_{cp} is the contribution to the HFF from the polarization of the s electrons of the inner shells of the zirconium atom by the magnetic moment of the zirconium atom, H_s is the contribution to the HFF from the polarization of the outer s electrons by the magnetic moment of the zirconium atom, and H_{sp} is the contribution to the HFF from the polarization of the conduction electrons by the magnetic moments of the nearest spheres. We shall investigate only the effect of the first and second CS on H_0. A zirconium atom in a $ZrFe_2$ lattice contains 12Fe in the first CS and 4Zr in the second CS. Since $H_{cp} + H_s$ is proportional to the magnetic moment μ_Z of the zirconium atom, we have $H_{cp} + H_s = H_{loc} = P_{Zr}\mu_{Zr}$, where P_{zr} is the intrinsic polarization constant for the zirconium atom. The contribution of each sphere to H_0 is proportional to the number N_i of the magnetic atoms and to the value of their magnetic moment μ_i (i is the number of the sphere: $H_{sp}^{(1)} = a_1N_1\mu_{Fe} = A_1\bar{\mu}_1$ and $H_{sp}^{(2)} = a_2N_2\mu_2 = A_2\bar{\mu}_2$ (where $N_1 = 12$Fe and $N_2 = 4$Zr, $\bar{\mu}_i$ is the average magnetic moment of the sphere i, while a_1, a_2, A_1 and A_2 are the constants of the polarization of the s electrons by the magnetic moments of the first and second CS). Equation (1) is written in the form

$$H_0=P_{Zr}\mu_{Zr}+a_1N_1\mu_{Fe}+a_2N_2\mu_{Zr}=P_{Zr}\mu_{Zr}+A_1\bar{\mu}_1+A_2\bar{\mu}_2. \quad (2)$$

No account is taken in this expresion of the dipole field (which we set equal to zero for the ZrF_2 cubic Laves phase) and of the Lorentz field. The Lorentz field is -24 kOe for $ZrFe_2$, and we shall take it into account in the HFF of the ^{91}Zr and impurity-atom nuclei.

The impurity atoms occupy in the $ZrFe_2$ lattice the sites of iron or zirconium atoms. It follows from Eq. (2) that the appearance of impurity atoms at the iron sites will perturb only the second term, leaving the others unchanged, and the appearance of these atoms at the zirconium sites perturbs the third term in Eq. (2) (assuming that the impurity atoms do not perturb the magnetic moments of the iron and zirconium atoms).

We consider first the influence of aluminum of the HFF H_0 of ^{91}Zr. Aluminum has no magnetic moment. Replacement of one iron atom by an aluminum atom in the first CS of zirconium shifts the HFF at the ^{91}Zr nuclei by 20.2 kOe. The difference between the HFF of ^{91}Zr whose atoms contain in the first CS 12Fe and 11Fe + 1Al yields directly the influence of the magnetic moment of one iron atom on the HFF of the ^{91}Zr nuclei. If the aluminum atoms in the first CS of the zirconium are replace by $3d$-element atoms, the difference between the HFF of ^{91}Zr with the nearest-atom configugration 11Fe + 1Z (Z stands here for Ti, V, Cr, Mn, Co, or Ni) and the HFF of ^{91}Zr atoms having 11Fe + 1Al in their first CS yields the effect of the magnetic moment of one transition element on the HFF. Since the corresponding contributions

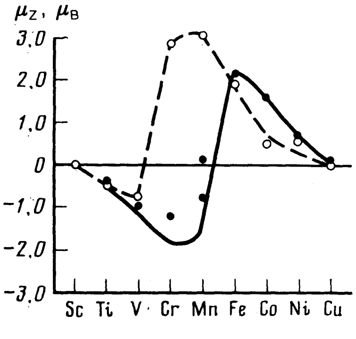

FIG. 3. Distribution of magnetic moments of $3d$ atoms in α-Fe matrices (● —experiment,[3] solid line—theory[1]) and $ZrFe_2$ (○ —NMR data, dashed line drawn for illustration).

to the HFF of ^{91}Zr are proportional to the magnetic moments μ_{Fe} and μ_Z of the nearest atoms, we obtain from Eq. (2), in analogy with Refs. 14 and 15, the relation

$$\frac{\mu_Z}{\mu_{Fe}}=\frac{H_0(11Fe+1Z)-H_0(11Fe+1Al)}{H_0(12Fe)-H_0(11Fe+1Al)}, \qquad (3)$$

where μ_Z is the local magnetic moment of the impurity atom, while μ_{Fe} is the magnetic moment of the iron atoms in the first CS of the zirconium atoms and is equal to $1.90\,\mu_B$[4,5] Relation (3) and the experimental HFF of the satellite peaks (see Table I) were used to calculate the magnetic moments at the impurity $3d$-element atoms in the intermetallic compound $ZrFe_2$. The table lists the values μ'_Z obtained in other studies. It can be seen that the data obtained by the NMR method and by the nuclear orientation method[7] and are in good agreement. A change from $Z=21$ (Sc) to $Z=29$ (Cu) changes the sign and the magnitude of the impurity-atom magnetic moment (see Fig. 3). The minimum of this oscillatory (s-shaped) curve corresponds to the vanadium atom ($Z=23$), and the maximum to chromium ($Z=24$) and manganese ($Z=25$). It can be seen from Fig. 3 that the magnetic-moment direction of the $3d$-element impurity atom changes from antiparallel to parallel (relative to the direction of the iron moment) on going from vanadium to chromium. Calculation of μ_Z from Eq. (3) at $\mu_{Fe} = 1/65\mu_B$ ($\mu_{Zr}=0$) does not alter the $\mu_Z(Z)$ dependence significantly; Thus for example, in this case we have $\mu_V = -0.73\mu_B$ and $\mu_{Mn} = +2.70\mu_B$.

We consider now the HFF at ^{45}Sc nuclei in a $ZrFe_2$ matrix. The scandium atoms occupy in the $ZrFe_2$ lattice zirconium-atom sites and contain 12Fe in the first CS and 4Zr in the second. The peak at 63 MHz corresponds to an impurity state of the scandium atoms with a hyperfine field $H_0 = -63.3$ kOe. Assuming that the HFF at the ^{45}Sc nuclei contain the same contributions as in Eqs. (1) and (2), we estimate separately the contributions $H_{loc} = P_{Sc}\mu_{Bc}H_{sp}$ to the HFF. The "scaling" method yielded in Ref. 17 an estimate -55 kOe for H_{sp} of the ^{45}Sc nuclei in $ZrFe_2$. This gives $H_{loc} = H_{exp} - H_{sp} = -7$ kOe. At $P_{Sc} = -55$ kOe/μ_B (Ref. 14) we obtain $\mu_{Sc} = (+0.12 \pm 0.10)\mu_B$. The error in the determination of μ_{Sc} is attributed to the uncertainties of the estimates of H_{sp} and P_{Sc}. Putting $P_{Sc} = -94$ kOe/μ_B for the atoms to the left of iron in the periodic table, we get from the estimate in Ref. 16 $\mu_{Sc} = 0.07\ \mu_B$ for impurities in Fe_3Si. The magnetic moment $\mu_{Sc} = (0.1 \pm 0.1)\mu_B$ agrees with the estimate of μ_{Sc} obtained from the HFF data by the nuclear-orientation method.[7] These estimates of the magnetic moment of the scandium atom show that it has probably no magnetic moment when it occupies a zirconium-atom site in $ZrFe_2$.

The HFF at the ^{65}Cu nuclei in a $ZrFe_2$ matrix is equal to -83 kOe. The sign of the field was taken from Ref. 7. Since no peaks whatever are resolved in the 40–45 MHz region of the NMR spectrum of ^{91}Zr in $ZrFe_2$ alloys containing copper-atom impurities, for the states of the zirconium atoms containing copper atoms in the first CS (or in the second CS), we shall likewise use the "scaling" method to estimate the local magnetic moment at the copper atoms. We express the HFF at the ^{65}Cu nuclei in the form $H_0 = H_{loc} + H_{sp}$. According to the estimates in Ref. 7, $H_{sp} = (-100 \pm 20)$ kOe for ^{65}Cu nuclei in $ZrFe_2$. Comparison on H_{exp} with H_{sp} shows that the HFF at the ^{65}Cu nuclei is determined only by the field due to polarization of the conduction s-electrons by the magnetic moments of the atoms of the nearest spheres, whereas $H_{loc} \approx 0$. The magnetic moment of copper in $ZrFe_2$ can thus be set equal to zero.

A theoretical analysis of the signs and magnitudes of the magnetic moments of the impurity atoms in iron was carried out in Ref. 1. The electronic structure of the impurity atom was calculated. These calculations resulted in values of μ_Z that agreed with the experimental data.[3] The solid line in Fig. 3 shows the theoretical plot of μ_Z. Comparison of the μ_Z curves for iron and $ZrFe_2$ shows that the transition from the ferromagnetic-iron matrix with a cubic lattice, $\mu_{Fe} = 2.2\mu_B$, and $T_C \approx 1000$ K to a ferromagnetic compound with a cubic structure, $\mu_{Fe} = 1.90\mu_B$, $\mu_{Zr} = -0.56\mu_B$ and $T_C = 630$ K shifts the μ_Z curve towards lower values of Z. The compound $ZrFe_2$ is so to speak some "effective" metal with an average magnetic moment $\bar{\mu} = 1.65\mu_B$ and $T_C = 630$ K (Ref. 7).

It follows from Table I and Fig. 1 that the position of the satellite resonance peak of the ^{91}Zr nuclei, whose atoms contain in the first CS $3d$-element atoms, is different from the magnetic moment of an impurity occupying iron-atom sites in the first CS of zirconium atoms. These data yield information on the dependence of the HFF $H_0^{(1)}$ at ^{91}Zr nuclei whose atoms have $11Fe + 1Z$ in the first CS, on the average magnetic moment μ_1 of the first CS. The values of the HFF for these satellites are given in Table I. The value of μ_1 was calculated for a first CS environment 12Fe or $11Fe + 1Z$ (where Z is the impurity atom). The magnetic moments for the atoms of the first CS are indicated in the table. The dependence of the HFF $H_0^{(1)}$ at the ^{91}Zr nuclei on the average magnetic moment μ_1 of the first coordination sphere is linear, $H_0^{(1)} = K_1 + A_1\mu_1$, in accord with Eq. (2). The slope of this straight line yields $A_1 = -(125 \pm 2)$ kOe/μ_B. Extrapolation of the values of H_0 to $\mu_1 = 0$ yields $K_1 = -(109 \pm 3)$ kOe. It follows from Eqs. (1) and (2) that $H_{sp}^{(1)} = A_1\bar{\mu}_1 = -237$ kOe and $H_{cp} + H_s + H_{sp}^{(2)} = 109$ kOe. Since the contribution made to the HFF by the second CS, which contains 4Zr, is much smaller than that of the first CS which contains 12Fe (with $\mu_{Zr} \ll \mu_{Fe}$), the existence of a nonzero positive field H_{loc} at the ^{91}Zr nuclei indicates that an appreciable negative moment is present at the zirconium atoms,[1)], thus confirming the conclusions of Ref. 4 and 5.

To estimate $\mu_{\rm Zr}$ from the data on the hyperfine fields and on the contribution of $H_{\rm loc}$ to the field at the ^{91}Zr nucleus in ZrFe$_2$, we must know the polarization constant $P_{\rm Zr}$ for the zirconium atom ($H_{\rm loc} = P_{\rm Zr}\mu_{\rm Zr}$). There are no published data on the constant $P_{\rm Zr}$ (as well as for many other d- and f-elements), and $P_{\rm Zr}$ can be estimated from the results of Ref. 1 on the hyperfine fields at ^{91}Zr nuclei and on the magnetic moment at the zirconium atom in an iron matrix. It is shown in Ref. 1 that $H_{\rm loc} \equiv H_{cp} = +80$ kOe for ^{91}Zr in iron with $\mu_{\rm Zr} = -0.4\mu_B$ Neglecting the contribution made to the hyperfine field of ^{91}Zr in ZrFe$_2$ from the polarization of the s electrons by the magnetic moment $\mu_{\rm Zr}$, under the assumption that $\mu_{\rm Zr}$ is much smaller than $\mu_{\rm Fe}$, we have $H_{\rm loc} \approx H_{cp} = +109$ kOe. We see that these contributions to the hyperfine fields at the ^{91}Zr nuclei in iron and in ZrFe$_2$ are practically equal. This indicates that the values of $\mu_{\rm Zr}$ in these matrices are also very close. From the data on Ref. 1 we get $P_{\rm Zr} = +80$ kOe$/(-0.4\mu_B) = -200$ kOe$/\mu_B$. With the aid of this value of $P_{\rm Zr}$ we estimate the magnetic moment $\mu_{\rm Zr}$ of the zirconium atom in ZrFe$_2$. It turns out to be $\mu_{\rm Zr} = +100$ kOe$/(-200$ kOe$/\mu_B) = -0.5\mu_B$. The accuracy of the estimates is $\approx 20\%$ or $\approx 0.1\mu_B$. This value of the magnetic moment of the zirconium atom agrees with the value $\mu_{\rm Zr} = -0.56\mu_B$ obtained in Ref. 4 from band calculations for ZrFe$_2$.

I am grateful to A. A. Sorokin, N. N. Delyagin, V. S. Shpinel', and V. I. Krylov of the Nuclear Physics Research Institute of the Moscow State University for a helpful discussion of the material in the paper.

[1] The contribution of the second CS to the HFF of ^{91}Zr in ZrFe$_2$ (from the magnetic moments of the zirconium atoms) will be considered in a later paper.

---

[1] H. Akai, M. Akai, and J. Kanamori, J. Phys. Soc. Jpn **54**, 4257 (1985).
[2] M. Akai, H Akai, and J. Kanamori, *ibid.* p. 4246.
[3] G. G. Low, Adv. Phys. **18**, 371 (1969).
[4] P. Mohn and K. Schwarz, Physica **B+C 130**, 26 (1985).
[5] S. T. Dumllow, P. C. Riedl, P. Mohn, K. Schwartz, and Y. Yamada, J. Mag. Magn. Mat. **54-57**, 1081 (1985).
[6] Handbook, "Phase Diagrams of Binary and Multicomponent Systems Based on Iron" [in Russian], Metallurgiya, 1986.
[7] J. Boysen, A. Heidari, and W. D. Brewer, J. Magn. Mat. **51**, 15 (1986).
[8] G. Wiesinger, A. Oppelt, and K. H. J. Buschow, *ibid.* **22**, 227 (1981).
[9] H. Nagai, H. Yoshie, and A. Tsujumura, J. Phys. Soc. Jpn **52**, 1122 (1983).
[10] V. S. Pokatilov. First All-Union Conf. on Nucl.-Spectrosc. Investigations of Hyperfine Interactions, Abstracts, Moscow, 1-3 Oct. 1985, p. 41.
[11] V. S. Pokatilov, V. V. Sadchikov, and O. V. Utenkova, Dokl. Akad. Nauk SSSR **281**, 574 (1985) [Sov. Phys. Dokl. **30**, 250 (1985)].
[12] V. S. Pokatilov, V. V. Dadchikov, E. F. Sidokhin, and O. V. Utenkova, Fiz. Met. Metallov. **62**, 69 (1986).
[13] M. Stearns, Phys. Rev. **B4**, 4081 (1971).
[14] A. Oppelt and K. H. J. Buschow, *ibid.* **B13**, 4698 (1976).
[15] Y. Yamada and K. Ohira, J. Phys. Soc. Jpn **50**, 3569 (1981).
[16] V. Niculescu, K. Raj, J. I. Budnick, T. J. Burch, W. A. Hines, and A. H. Menotti, Phys. Rev. **B14**, 4160 (1976).

Translated by J. G. Adashko