

*MAGNETIC HYPERFINE INTERACTION FOR TIN ATOMS IN METALLIC FERRO-
AND ANTIFERROMAGNETS WITH BCC STRUCTURE*

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The magnetic hyperfine fields for impurity Sn atoms in ferromagnetic ordered Fe₃Si and Fe₃Al alloys are measured by means of the Mossbauer effect for Sn¹¹⁹ nuclei. At a temperature of 77°K the field strengths in the two matrices are found to be -50.0 ± 1.5 and $+8.5 \pm 1.5$ kOe, respectively. The field temperature dependences are close to the temperature dependences of the Fe⁵⁷ hyperfine fields in the same alloys. It is shown that the experimental data on magnetic hyperfine fields for Sn atoms in metallic ferro- and antiferromagnetic substances with bcc structures can be represented by a simple formula which relates the field strengths to the distribution of the matrix-atom magnetic moments over the coordination spheres. The partial contributions to the hyperfine field from various coordination spheres are proportional to the mean atomic magnetic moment of the sphere and can be regarded, with good accuracy, as constant quantities independent of details of the matrix electron structure. The negative contribution to the hyperfine field in this case is determined mainly by the immediate neighbors of the Sn atom, whereas the positive contribution is due mainly to the matrix atoms in the more remote coordination spheres. Some features of magnetic hyperfine interaction for nonmagnetic atoms in magnetic matrices are discussed in connection with regularities found on the basis of the model proposed in [3].

1. INTRODUCTION

THE interpretation of the data on magnetic hyperfine fields in ferro- and antiferromagnetic metals and alloys is a complicated and far from solved problem. The theoretical calculation of the hyperfine fields can be carried out only on the basis of very crude models, which simplify the real situation excessively. Moreover, it cannot be assumed that the main factors on which the hyperfine field depends have been uniquely determined.

In the present article we consider the magnetic hyperfine interaction only for nonmagnetic atoms, i.e., for atoms having no magnetic moment of their own. In this case it is usually assumed that the occurrence of the magnetic hyperfine field is due to the interaction between the nonmagnetic atom and the polarized conduction electrons of the matrix, [1-4] but frequently the experimental data are also explained by employing the mechanism of direct overlap of the nonmagnetic-atom electrons with the magnetic electrons of the matrix atoms. [5] Even if we confine ourselves to the mechanism wherein the polarization is transferred via the conduction electrons, there are still unanswered questions connected with the influence exerted on the hyperfine field by such factors as the electron concentration, the density of states, the structure of the electronic wave functions at the Fermi surface, etc. In most cases [1,2,4] it is traditional to consider only the direct contact interaction of the nucleus with the conduction electrons, but in [3] there are arguments in favor of a contact interaction with the polarized electrons of the internal shells of the nonmagnetic atom. The distinct progress made recently towards understanding the nature of magnetic hyperfine fields in metallic matrices is connected mainly with empirical and semiempirical models, [1-5]

but the development of these models has not led so far to the formation of a unified approach to the interpretation of the experimental data.

The models proposed in [1-4] do not consider the radial dependence of the conduction-electron polarization, and therefore are applicable only to an isolated impurity atom in a homogeneous magnetic matrix. New problems arise when the magnetic hyperfine interaction is considered in alloys, when the distribution of the atomic magnetic moments over the coordination spheres is not uniform. An analysis of the experimental data for ordered alloys (intermetallides) calls for an explicit allowance for the radial dependence of the exchange interaction, inasmuch as the hyperfine field should be determined not so much by the average polarization of the conduction electrons in the alloy as by the polarization near the atom in question. Assuming that the degree of polarization of the conduction electrons is proportional to the atomic magnetic moments, it is therefore necessary to take into consideration the distribution of these moments over the nearest coordination spheres relative to the given atom.

The radial dependence of the conduction-electron polarization was considered in explicit form in the well known RKKY (Ruderman-Kittel-Kasuya-Yosida) theory [6] and the model of Caroli and Blandin. [7] Unfortunately, calculations in accordance with the RKKY theory or the Caroli-Blandin model can be performed in practice only for idealized systems whose properties have been simplified to the utmost compared with real ferromagnets. The difficulties that arise in the RKKY theory when a more realistic account is taken of the properties of the electrons in the conduction band have been considered in detail in Watson's review. [8] In such a situation, one should call attention to the possibility of an empirical approach to the consideration of the radial dependence

of the exchange interaction that determines the hyperfine magnetic field for a nonmagnetic atom in a metallic ferro- or antiferromagnet.

Certain peculiarities of the radial dependence of the contributions made to the hyperfine field were considered for Sn atoms in ^[8], on the basis of a model proposed in ^[9]. According to this model, the hyperfine magnetic field for a nonmagnetic atom is an algebraic sum of two large contributions of opposite sign. For Sn atoms these contributions are close in absolute magnitude, and therefore the observed values of the fields for Sn are relatively small and very sensitive to the distribution of the magnetic moments of the atoms of the matrix over the coordination spheres. It was shown in ^[8] that many experimental data can be explained from a unified point of view, assuming different radial dependences for the positive and negative contributions to the hyperfine field. According to this assumption, the negative contribution is to a greater degree "local" than the positive one, since the latter is determined by a larger number of coordination spheres. This conclusion is in good agreement with the correlation found in our earlier investigation^[8,9] between the values of the magnetic hyperfine field for Sn and the distribution of the magnetic moments of the matrix atoms over the coordination spheres. In the present paper, we consider, from this point of view, the experimental data on magnetic hyperfine fields for Sn atoms in ordered metallic ferro- and ferromagnets with bcc structure.

In Sec. 2 we present new results obtained with the aid of the Mossbauer effect for Sn¹¹⁹ impurity atoms in the alloys Fe₃Al and Fe₃Si. Section 3 is devoted to an analysis of all the available data on magnetic hyperfine fields for Sn in magnetic metallic matrices with bcc structure. It will be shown that these data can be represented with good accuracy by a simple formula that relates the field with the distribution of the magnetic moments of the matrix atoms over the coordination spheres. In the same section we present an interpretation of the experimental results for Sn¹¹⁹ in Fe₃Al and Fe₃Si matrices. In Sec. 4 we discuss certain consequences from the laws obtained for magnetic hyperfine fields.

2. MAGNETIC HYPERFINE FIELDS FOR Sn¹¹⁹ IMPURITY ATOMS IN ORDERED Fe₃Al AND Fe₃Si ALLOYS

The ordered ferromagnetic alloys Fe₃Al and Fe₃Si have a bcc (DO₃) structure, which can be represented in the form of two mutually penetrating primitive cubic sublattices, one of which contains Fe atoms (Fe I) and Al or Si atoms, while the other contains only Fe atoms (Fe II). The atomic magnetic moments in these alloys are determined by the method whereby the neutrons are scattered.^[10] The magnetic moments for the atoms Fe I and Fe II are respectively (in μ_B) 2.18 ± 0.10 and 1.50 ± 0.10 in Fe₃Al and 2.40 ± 0.06 and 1.20 ± 0.12 in Fe₃Si. The moments of the Al and Si atoms are negligibly small or equal to zero. The hyperfine interaction in these alloys, for Fe⁵⁷ atoms, were investigated with the aid of the Mossbauer effect by a number of workers (see, for example, ^[11]).

We prepared ordered Fe₃Al and Fe₃Si alloys for our measurements with a small admixture of Sn enriched to

85.2% of Sn¹¹⁹. The samples were obtained by fusion in vacuum and were homogenized at 1000°C for 20–40 hours. The ingots were ground into powders which were then annealed under conditions ensuring production of an ordered structure. The quality of the alloys was monitored by measuring the absorption spectra for Fe⁵⁷; for well-ordered alloys the results of these measurements agree with the data of ^[11]. A preliminary investigation was made of samples with different Sn concentrations. It was established that the solubility of Sn in the ordered Fe₃Si alloy is very small, namely, a line corresponding to the nonmagnetic phase was observed in the absorption spectra of Sn¹¹⁹ at Sn concentrations exceeding 0.2 at.%. The main measurements were made with the Fe₃Si alloy containing 0.15 at.% Sn, for which the admixture of the nonmagnetic phase was negligibly small. It was also found that the mechanical working accompanying the preparation of the powders from the Fe₃Si ingots does not influence the form of the absorption spectrum and consequently does not affect significantly the ordered structure of the alloy.

For Fe₃Al, the solubility of Sn was higher: the form of the absorption spectrum was practically independent of the Sn concentration, at least up to 0.4 at.%. At the same time, the form of the absorption spectrum for Sn¹¹⁹ in Fe₃Al turned out to be quite sensitive to the stoichiometry of the alloy and to the mechanical working, in that the spectra for samples of nonstoichiometric composition and for nonannealed powders contained lines corresponding to the disordered structure. (It can be noted that these results agree with the data obtained for Fe₃Al by the NMR method^[12].) The main measurements were performed with ordered Fe₃Al samples containing 0.30–0.35 at.% of Sn, at deviations from stoichiometry not exceeding 0.5 at.%. The procedure for the measurement of the Mossbauer absorption spectra was analogous to that employed in ^[9]; the sign of the hyperfine field was determined by measurements of the absorption spectra in external magnetic fields of intensity from 2.5 to 16 kOe. The experimental spectra were compared with the theoretical ones calculated with a BESM-4 computer.

Typical absorption spectra are shown in Fig. 1. For Fe₃Si(Sn), the form of the absorption spectrum indicates that there is one value of the hyperfine field, i.e., the Sn¹¹⁹ atoms occupy sites of the same type in the ordered Fe₃Si alloy (as was the case, for example, also for Sn¹¹⁹ atoms in the FeRh alloy^[9]). The best agreement between the experimental and theoretical spectra was obtained when the width of each component of the hyperfine struc-

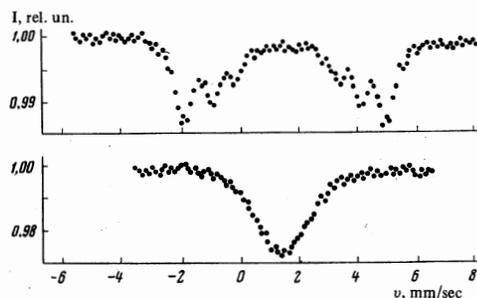


FIG. 1. Absorption spectra for Sn¹¹⁹ in Fe₃Si (upper figure) and Fe₃Al (lower figure) at 77°K. Abscissas—velocity of γ -quantum source, ordinates—intensity of quantum flux in relative units.

ture was 0.80 ± 0.05 mm/sec, which is close to the natural line width for the 23.8-keV γ radiation of Sn^{119} . For $\text{Fe}_3\text{Al}(\text{Sn})$, the magnitude of the hyperfine field is small and the components of the hyperfine structure are not resolved, but in this case good agreement between the experimental spectra and the theoretical ones was obtained assuming that one value of the hyperfine fields exists. The widths of the hyperfine-structure components equaled in this case 1.14 ± 0.10 mm/sec (at 77°K). The increased width is apparently due to small deviations of the ordered structure of the alloy from ideal. The widths of the hyperfine-structure components decrease with increasing temperature, approaching 0.8 mm/sec near the Curie temperature. Measurements in external magnetic fields have shown that the hyperfine field for Sn^{119} impurity atoms is negative in the Fe_3Si matrix and positive in Fe_3Al . These measurements have also confirmed that the form of the spectrum for $\text{Fe}_3\text{Al}(\text{Sn})$ can be interpreted with sufficient accuracy as a result of magnetic hyperfine interaction at one value of the hyperfine field. The values of the hyperfine fields at 77°K were found to be -50.0 ± 1.5 kOe for Sn^{119} in Fe_3Si and $+8.5 \pm 1.5$ kOe for Sn^{119} in Fe_3Al . The temperature dependences of the fields for Sn^{119} turned out to be quite close to the temperature dependences of the hyperfine fields for Fe^{57} in the same alloys (without the Sn impurity), as measured in [11]. For the Fe_3Al alloy, however, this result was established only approximately, since the dependence of the widths of the hyperfine structure components on the temperature could not be determined with sufficient accuracy. For $\text{Fe}_3\text{Si}(\text{Sn})$, the temperature dependence of the hyperfine field is shown in Fig. 2.

For an interpretation of the measurement results it is necessary to identify precisely the sites occupied by the Sn atoms in the Fe_3Al and Fe_3Si structures, but this cannot be done only on the basis of the experimental data obtained here. The results will be interpreted in the next section, after we obtain a relation between the hyperfine field for Sn in bcc structures and the distribution of the magnetic moments of the matrix atoms over the coordinate spheres.

3. FORMAL ANALYSIS OF THE MAGNETIC HYPERFINE FIELDS FOR Sn IN METALLIC FERRO- AND ANTIFERROMAGNETS WITH BCC STRUCTURE

Let us assume that for a nonmagnetic atom in a magnetic matrix the contributions made to the hyperfine field by each of the coordination spheres are additive

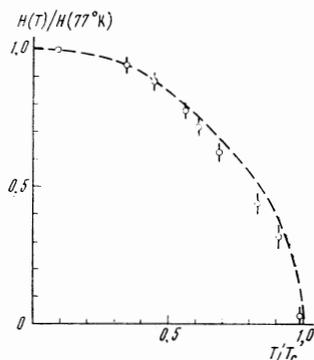


FIG. 2. Temperature dependence of the magnetic hyperfine field H for Sn^{119} in a Fe_3Si matrix. The dashed line shows the temperature dependence of the magnetic hyperfine field for Fe^{57} as measured in [11].

and proportional to the magnetic moments of the matrix atoms in the given coordination sphere. We can then write for the hyperfine field H the following general expression:

$$H = \sum_{i=1}^{\infty} h_i n_i \mu_i, \quad (1)$$

where i is the number of the coordination sphere, n_i the number of the atoms in the i -th sphere, μ_i the average magnetic moment per atom in the i -th sphere (in μ_B), and h_i the partial contribution made to H per Bohr magneton for the i -th sphere. For the structures of the given type (in our case, bcc), the values of n_i are known and are the same for all systems.

The quantities h_i can be regarded as experimentally determined parameters. The limited amount of experimental data makes it possible to determine only a small number of parameters, and therefore formula (1) must be significantly simplified. It is clear from general considerations that the series in formula (1) is indeed finite, inasmuch as the partial contributions h_i should become negligibly small at sufficiently large i , but it is not known beforehand how many spheres must be taken into account. In the simplest variant one takes into account in explicit form only the contribution from the first sphere, and the contributions from the remaining spheres are averaged out; such an approximation was used in fact in [8,9]. In the bcc structure, the first two coordination spheres, which lie close to each other, are geometrically singled out, and it is therefore natural to take explicit account of the contributions from these two spheres, writing the formula for H in the form

$$H = a\mu_1 + b\mu_2 + c\bar{\mu}, \quad (2)$$

where $a = h_1 n_1$, $b = h_2 n_2$ and c are empirical coefficients, while c is the average atomic magnetic moment of the matrix. The experimental data obtained to date make it possible to determine with sufficient reliability the three empirical parameters of this formula. If we take into consideration the rapid decrease of the partial contributions h_i with increasing distance (or, equivalently, with increasing number of the sphere i), then it is natural to modify somewhat the last term in formula (2), averaging the contributions from the spheres with $i \geq 3$ not over the entire crystal but over a finite number of spheres (from $i = 3$ to $i = m$, where m is the number of the last sphere taken into account). Such a variant might be of considerable interest (from the point of view of determining the effective radius of the exchange interaction), but for the systems considered below the results of the analysis of the experimental data turned out to be little sensitive to the choice of m , and we therefore confine ourselves for simplicity to a discussion of formula (2), which corresponds to the case $m = \infty$.

It should be noted that formulas (1) and (2) can be of practical value only if the partial contributions h_i (or the coefficients a , b , and c) are the same with good accuracy in different systems (within the limits of one type of structure). This does not follow in any manner from general considerations, since the quantities h_i , generally speaking, can depend in a complicated manner, say, on the singularities of the electronic structure of the matrix. One of the most important results of the

analysis that follows is the conclusion that the partial contributions h_i are actually constants with good accuracy and are little sensitive to individual properties of the alloys.

To determine the coefficients of formula (2), we consider systems for which there exist sufficiently reliable data on the atomic magnetic moments and the magnetic hyperfine fields for Sn atoms; these data are listed in Table I. The values of H for Sn vary in a wide range, and it is easy to see that H is determined not so much by the absolute values of the magnetic moments as by their distribution over the coordination spheres. (Characteristic examples are the two radically different values of H in the CoFe matrix and the relatively large H in antiferromagnetic chromium.) Using the data of Table I, we obtain the coefficients of (2) with which this formula best describes the experimental values of H. The coefficients were found to be (in kOe/ μ_B):

$$a = -218, \quad b = +9, \quad c = +165 \quad (3)$$

The values of H calculated from formula (2) with the coefficients (3) are also given in Table I. We see that in no case does the difference between the experimental and calculated values of H exceed 20 kOe, which should be regarded as very good agreement, in view of the simplicity and certain approximateness of formula (2), and also in view of the not too high accuracy of the known values of the atomic magnetic moments for certain systems.

The possibility of representing the experimental data quite accurately by means of the simple formula (2) with the coefficients (3) enables us to draw the following fundamental conclusions:

1. The contributions to the hyperfine magnetic field from different coordination spheres are additive with good accuracy and are proportional to the average atomic magnetic moments of each of the spheres; the partial contributions h_i are not very sensitive to singularities of the electronic structure of the matrices.

2. In connection with the hypotheses advanced in [8,9], the nearest neighbors of the Sn atom make a large negative contribution to the hyperfine field, while the more remote neighbors make a positive contribution. The contribution from the second coordination sphere is relatively small.

3. The coefficients a and c of formula (2) for Sn are close in absolute magnitude, and therefore the values of

H are determined primarily by the relation between μ_1 and $\bar{\mu}$. Obviously, in this case the sign and the absolute magnitude of H cannot be directly compared with the sign and magnitude of the average electron polarization in the conduction band of the matrix.

Certain consequences of the obtained regularities will be considered in the concluding section of the article.

Formula (2) with coefficients (3) makes it possible to explain the experimental data obtained in the present investigation for Fe₃Al and Fe₃Si matrices. In Table II, the experimental values of H for Sn in these matrices are compared with the values calculated from formula (2) for three nonequivalent lattice sites. We see that in both cases the experimental values of H are in good agreement with the calculated values for the Fe II sites (within an interval of 20 kOe, which, as noted above, characterizes the accuracy of the empirical formula). For the Fe₃Al matrix we can state with assurance that the Sn impurity atoms occupy Fe II sites, since the calculated values of H for the first two sites differ strongly from the experimental value. For the Fe₃Si matrix within the limits of the assumed 20 kOe accuracy, the experimental value of H agrees with all three calculated values, so that it is impossible to draw an unambiguous conclusion concerning the localization of the impurity atoms, but nonetheless the best agreement is likewise obtained for an Fe II site, i.e., for the sublattice containing only Fe atoms. (We note that a similar character of the localization of the Sn impurity atoms was observed in the ordered alloy FeRh, where the Sn impurity atoms occupied sites only in the Fe sublattice.^[9])

4. DISCUSSION OF EXPERIMENTAL REGULARITIES

For a qualitative interpretation of formula (2), we use the model proposed in [3], according to which the magnetic hyperfine field H for a nonmagnetic atom in a magnetic matrix can be represented in the form

$$H = -H^- + H^+, \quad (4)$$

i.e., as the algebraic sum of two large contributions of comparable magnitude and of opposite sign.

In the general case we should assume that each of the partial contributions h_i is a sum

$$h_i = -h_i^- + h_i^+ \quad (5)$$

i.e., $H^- = \sum h_i^-$ and $H^+ = \sum h_i^+$. For the atoms of the first coordination sphere $h_1^- > h_1^+$, and therefore the partial

Table I. Magnetic hyperfine fields H for Sn atoms in metallic ferro- and antiferromagnets with bcc structure

Matrix	Site occupied by the Sn atom	μ_1	μ_2	$\bar{\mu}$	H, kOe	
					experiment	calculation from formula (2)
Fe	Fe	2.2	2.2	2.2	-83 [8,19]	-97
Cr	Cr	0.4	-0.4	0.0	-98 [14]	-91
FeRh	Fe	1.0	3.1	2.05	+147 [9]	+148
Co ₂ MnSn	Sn	0.7	4.0	1.35	+106 [15]	+106
CoFe	Co	3.0	1.85	2.43	-252 [16]	-237
CoFe	Fe	1.85	3.0	2.43	+7 [16]	+24

Note. μ_1 , μ_2 , and $\bar{\mu}$ are the average magnetic moments of the atoms of the matrix for the first and second coordination spheres and for the entire matrix, respectively. The sign of the hyperfine field for Sn in antiferromagnetic Cr is indicated relative to the orientation of the magnetic moments of the matrix atoms in the first coordination sphere for the phase AF₀.

Table II. Comparison of experimental magnetic hyperfine fields H for Sn^{119} in Fe_3Al and Fe_3Si matrices with those calculated from formula (2)

Matrix	Site occupied by the Sn atom	μ_1	μ_2	$\bar{\mu}$	H, kOe	
					calculation from formula (2)	experiment
Fe_3Al	FeI	1.5	0	1.29	-114	—
	FeII	1.09	1.5	1.29	-11.5	$+8.5 \pm 1.5$
	Al	1.5	2.18	1.29	-95	—
Fe_3Si	FeI	1.2	0	1.2	-64	—
	FeII	1.2	1.2	1.2	-53	-50.0 ± 1.5
	Si	1.2	2.4	1.2	-42	—

contribution h_1 is negative. The exchange interaction responsible for the negative contribution to the hyperfine field decreases rapidly with distance, so that the positive contribution begins to predominate even for the second sphere. The positive partial contributions, of course, also decrease with increasing distance, but more slowly than the negative ones. A possible dependence of h_1^- , h_1^+ , and h_1 on the distance is shown schematically in Fig. 3. According to [3], the negative contribution H^- in the homogeneous matrix is a simple function of the nominal number of outer electrons of the nonmagnetic atom, a fact that can be attributed, for example, to the formation of quasibound states of the conduction electrons in the impurity-atom potential (see also [1]). The positive contribution H^+ does not depend on the number of outer electrons and is interpreted in [3] as a result of direct interaction of the conduction electrons with the electrons of the filled shells of the nonmagnetic atom. Such a difference between the mechanisms governing the two contributions to the field may explain the strong difference between the radial dependences of the corresponding exchange interactions.

In the case when the first coordination sphere is nonmagnetic, the hyperfine field for the Sn atoms should always be positive. This conclusion makes it possible, in our opinion, to explain in natural fashion the result of the experiment of Nikolaev et al. [17] for sandwiches made by successive sputtering of Sn and Fe layers. In such samples, the overwhelming majority of the Sn atoms have no magnetic atoms among their nearest neighbors and one should expect the hyperfine fields for Sn to be positive, as was indeed experimentally observed. It should be noted, however, that the results of these measurements still do not give grounds for drawing definite conclusions concerning the sign of the polarization of the conduction electrons in Fe, since the mechanism whereby the nonmagnetic atom interacts with the polarized conduction electrons cannot be regarded as established.

The regularities considered above should become manifest in magnetic hyperfine interactions not only for

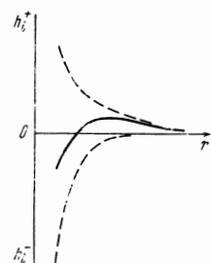


FIG. 3. Possible form of the radial dependence of the partial contributions to the magnetic hyperfine field h_1^- , h_1^+ (dashed lines) and h_1 (solid line) for Sn atoms. The ordinate scale is arbitrary.

the Sn atoms, but also for other nonmagnetic atoms, but it is precisely for Sn that these regularities are especially strongly pronounced, since, as already noted, for Sn the contributions of H^- and H^+ are very close in magnitude. According to the results of [3] for atoms located to the right of Sn in the periodic table, H^+ greatly exceeds H^- , whereas for atoms located to the left of Sn, to the contrary, H^- prevails. Nonetheless, even for these atoms, at substantial deviations from uniform distribution of μ_i over the coordination spheres, one should expect abrupt changes in the values of the hyperfine fields. An analysis of the hyperfine fields in ordered structures for other nonmagnetic atoms would be of great interest, but at present we still do not have the experimental data required for this purpose.

Attention should be called to the fact that the results obtained here do not confirm the assumption made in [5] that the positive fields for the elements at the end of period V (Sn–Xe) are due to the direct overlap mechanism. Were this assumption correct, the partial contribution from the coordination sphere would be positive, in contradiction to the experimental data. The result of [13], where an increase of the negative field for the Sn was observed in the Fe matrix under pressure, should likewise not be regarded as evidence in favor of the direct overlap mechanism. This result can be attributed to the sharp radial dependence of the negative contribution to the field, which increases with decreasing interatomic distance.

We note that an opposite effect should be observed for Sn impurity atoms in an Ni matrix, where the hyperfine field is positive. The increase of the negative contribution upon compression of the matrix should in this case lead to a decrease of the observed hyperfine field for Sn atoms.

In the analysis of the experimental data in Sec. 3 we did not take into account the possible change of the partial contributions h_1 as a result of the differences in the interatomic distances in different matrices, since the functional form of such a correction is unknown. For all matrices represented in Table I, however, these distances are the same accurate to about 3%; it can be assumed that in this case the influence of the differences between the interatomic distances does not exceed the accuracy limits of the empirical formula. In those cases when changes of the interatomic distances turn out to be appreciable, one should expect an appreciable change in the ratio of h_1^- to h_1^+ , which in turn changes the coefficients of the formula (2). This change will apparently be particularly appreciable for the partial contribution made to the field by the first coordination sphere.

In conclusion, we note that the regularities considered above should be valid not only for matrices with bcc structure, but also for metallic ferro- and antiferromagnets with arbitrary structure. Of course, the coefficients of empirical formulas such as (2) will be different here, since they depend on the number of atoms in the coordination spheres and on the distances, i.e., on quantities that vary from structure to structure. At the same time, one should expect that at a fixed distance, the partial contributions per atom, h_1/n_i , should be approximately the same for all structures. In the bcc structure, the first coordination sphere contains eight atoms, and therefore the partial contribution per Bohr

magneton from one atom in this sphere is approximately -27 kOe.

In fcc structures such as Co or Ni, the distance from a given atom to the atoms of the first coordination sphere is practically the same as for the considered bcc structures, and therefore the partial contribution per atom for the first coordination sphere should be the same in both types of structures. Recognizing that in fcc structures the first coordination sphere contains 12 atoms, one should expect the coefficient of μ_1 in the empirical formula for fcc matrices to be close to -320 kOe. This does not mean, however, that in fcc structures the ratio of the positive and negative contributions to the magnetic hyperfine field changes significantly in favor of the latter. In fcc structures, as compared with bcc structures, there is a simultaneous increase of the density of the atoms located in the more remote spheres. This leads (at a specified exchange-interaction radius) to the corresponding increase of the positive contribution to the hyperfine magnetic field. As a result, for most impurity nonmagnetic atoms in homogeneous metallic matrices (Fe, Co, Ni), the values of the hyperfine fields turn out to be approximately proportional to the atomic magnetic moment of the matrix, in spite of the differences between the crystal structures of the matrices.

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