Magnetic hyperfine interaction of ^{119}Sn impurity atoms in ordered alloys of iron with palladium and platinum. Radial dependence of the partial contributions to the magnetic hyperfine field

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Mössbauer spectroscopy is used to investigate the magnetic hyperfine interaction for ^{119}Sn impurity atoms that replace Fe atoms in the ordered ferromagnetic alloys $FePd_3$ and Fe_3Pt and in the antiferromagnetic alloy $FePt_3$. The magnetic hyperfine fields for the Sn atoms at 77 K are found to be $+9.1 \pm 0.2T(FePd_3)$, $\pm 0.07 \pm 0.03T(Fe_3Pt)$, and $8.0 \pm 0.3T(FePt_3)$. The results are interpreted with the aid of an empirical function $p(r)$ of the radial dependence of the partial contributions to the hyperfine field, obtained by a combined analysis of the data for 16 metallic ferromagnetic matrices. The characteristic features of the function $p(r)$ are: a sharp radial dependence of the negative partial contributions in the region $r = 2.5$–2.8 Å, a reversal of the sign at $r = 2.9$–3.2 Å, and a large positive maximum at $r \approx 3.5$ Å. The possibility of interpreting a large group of data with the aid of a single function $p(r)$ confirms the weak dependence of the partial contributions on the structure and on the composition of the alloys. Attention is called to the qualitative similarity of the $p(r)$ functions obtained for the atoms Sn and Fe.

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1. INTRODUCTION

Definite progress was made in recent years in the experimental and theoretical studies of the magnetic hyperfine interactions (MHI) of nonmagnetic atoms in metallic magnets. The interest in this problem is due, in particular, to its direct connection with certain general aspects of the electron theory of magnetic metals. At the same time, this connection makes the problem complicated, and it is therefore not surprising that the theoretical MHI models are still far from perfect. It must be emphasized that the difficulties of the theory are not so much quantitative as qualitative, since there is a considerable arbitrariness in the choice of those interaction mechanisms which are assumed to be essential for the formation of the magnetic field in the region of the nucleus of a nonmagnetic atom.

A nonmagnetic atom does not have a magnetic moment of its own, so that the magnetic field in the region of the nucleus of such an atom is determined by the magnetic environment. The problem is thus to ascertain the mechanism whereby a nonzero spin density (electron polarization) is transferred from the magnetic environment to the nonmagnetic atom. There is no meeting of minds concerning the number and type of these mechanism, and the MHI models proposed by different authors are contradictory in some of their basic premises.

For example, in the models of Blandin and Campbell[1] and of Jena and Geldart[2] the only source of the hyperfine field is the Fermi contact interaction with the polarized conduction electrons, and the magnitude and sign of the field are determined by the parameters of the nonmagnetic-atom potential. At the same time, to explain the same experimental data, Stearns[3] considers in his model two independent contributions to the hyperfine field: the Fermi contact interaction, and the "volume contri-

bution" due to the overlap of the electron wave functions of the neighboring atoms. The dependence of the spin density on the nonmagnetic-atom potential is not considered in this model at all. These examples show that the contradictions between the different models are quite far-reaching. Each of the models is vulnerable to criticism, but the experimental data at our disposal do not give sufficient grounds for an objective choice of a model or even for an unequivocal determination of the number of independent contributions to the magnetic field.

Similar difficulties and contradictions arise in the analysis of the important problem of the radial dependence of the spin density (RDSD) in a metallic magnet. In general form, the magnetic hyperfine field H for a nonmagnetic atom is the sum of the contributions from all the neighboring atoms:

$$H = \sum m_i(r_i) p(r_i), \tag{1}$$

where m_i is the magnetic moment of the i-th magnetic atom located at a distance r_i (in units of μ_B), and $p(r_i)$ is a distance-dependent partial contribution to H (in units of T/μ_B). It follows from this equation that knowledge of the function $p(r)$ is of prime importance for the interpretation of the experimental data. The form of this function, of course, depends on the type of interaction that determines the partial contributions to H. If, for example, it is assumed that the source of H is contact interaction with the conduction electrons, then from the theoretical point of view the determination of the function $p(r)$ is equivalent to the calculation of the RDSD in the conduction band. Various approximations are used for this purpose. For example, in the Caroli-Blandin model[4] are considered the spin-density oscillations due to virtual bound states of the d electrons of the magnetic atom. The model cannot be

used at short distances and fails to take into account the dependence of the spin density on the potential of the nonmagnetic atom. The calculation of the RDSD in the Blandin-Campbell model[1] is based on the classical RKKY (Ruderman-Kittel-Kasuya-Yosida) theory; the effect of the nonmagnetic-atom potential is taken into account by introducing an additional phase shift of the spin-density oscillations. In calculations of the RDSD on the basis of the d-resonance theory (see, e.g., Ref. 5), the properties of the "real" d-electron wave functions are taken explicitly into account, therefore the results are valid for all distances between the atoms. Yet the difficulties connected with allowance for the nonmagnetic-atom potential persists also in this theory. Finally, Stearns[3] introduces in his model a superposition of RKKY oscillations and interband mixing.

All the RDSD models involve parameters that cannot be determined in experiment; this makes a direct comparison of the theory and the experimental data difficult. The RDSD calculations are usually made in the free-electron approximation, which is a great over-simplification of the real situation in d-metal alloys. Strictly speaking, the results of the calculation are valid only for an isolated magnetic atom in a metal with a simple electron structure. The extent to which these results are applicable to concentrated magnetic alloys remains unclear.

Obviously, an experimental determination of the function $p(r)$ would be extremely helpful for a check on the MHI model as well as for an interpretation of concrete experimental results. Unfortunately, the partial contributions $p(r_i)$ can be measured only in isolated individual cases. A good example of such measurements are the Stearn's results[3,6] obtained for Fe atoms. No such data are available as yet for nonmagnetic atoms in alloys of transition d metals.

It is therefore vital to have another method of empirically determining $p(r_i)$, based on a comparison of the data for a large number of systems with substantially different distributions of the magnetic moments over the coordination spheres. The success of such an approach to the analysis of experimental depends on whether or not the function $p(r)$ (for a given nonmagnetic atom) is universal to one degree or another, i.e., whether it is the same for a large group of ferromagnetic alloys. An affirmative answer to this question turns out to be diametrically opposite, depending on whether the statement is made on the conclusions of theoretical models or on the experimental data. The theoretical RDSD models predict as a rule a strong dependence of the function $p(r)$ on the details of the electron structure of the magnet, since the form of this function is determined by parameters such as the electron density, the wave vector on the Fermi surface, the exchange-splitting energy, the width and position of the virtual bound state, and others. These parameters are greatly different for alloys with different compositions and with different structures, so that each case calls for a concrete calculation of the RDSD with allowance for the distinguishing features of the electron structure of the given system.

The results of an analysis of the experimental data do not confirm this point of view and are in this sense more optimistic. In a number of cases, simple empirical relations are obtained that are valid for a large group of magnetic systems. The simplicity and generality of these relations point to a weak dependence of H on the foregoing parameters that characterize the electron structure of the alloy. For example, the data for Sn atoms in magnets with bcc structure can be represented by a simple empirical formula,[7] according to which the magnitude and sign of H are determined primarily by the distribution of the magnetic moments over the coordination spheres. The correctness of this formula must be regarded as a confirmation of the relative independence of the function $p(r)$ of the electron density and of the type of magnetic atoms in the alloy. The obtained relations have made it possible to explain from a single point of view the dependences of H on the temperature[8] and on the pressure,[9] as well as the variations of H in certain isostructural ferromagnets.[10] It is also well known[11] that the influence of nonmagnetic impurity atoms in the MHI in metallic iron is practically independent of the valence of the impurity. Stears has recently shown[12] that in ferromagnetic Geissler alloys the partial contributions for different nonmagnetic atoms are independent of the electron density.

These data show that the search for a universal (for a definite type of nonmagnetic atom) function $p(r)$ is well justified. At any rate, the results of such an attempt can be regarded as a method of empirically describing the experimental data, that permits a determination of certain important properties of the function $p(r)$. In Sec. III of this article we consider the data obtained on the radial dependence of $p(r)$ by analyzing the experimental data for Sn atoms in metallic ferromagnets with bcc, fcc, and hcp structures. The empirical functions $p(r)$ are used in Sec. IV to interpret the new data on the MHI impurity Sn atoms in ordered alloys of Fe with Pd and Pt, as well as other previously obtained data.

II. MAGNETIC HYPERFINE FIELDS FOR IMPURITY Sn ATOMS IN THE ORDERED ALLOYS FePd$_3$, Fe$_3$Pt, AND Fe$_3$Pt

The experimental data on MHI for Sn atoms do not include any data for systems with fcc structure. To fill this gap to some degree, we have investigated by Mössbauer γ spectroscopy the MHI for ^{119}Sn impurity atoms in three ordered alloys with fcc structure of the Cu$_3$Au type: in the ferromagnetic alloys FePd$_3$ and Fe$_3$Pt and in the antiferromagnetic alloy FePt$_3$.

The alloys were obtained by fusing the components (of purity not worse than 99.98%) in high vacuum; tin enriched with ^{119}Sn to 91% was first added to the iron. To increase their homogeneity, the ingots were remelted three times and then annealed at 1000 C for 70 hr. The melting losses did not exceed 0.3 wt.%, so that the component concentration (disregarding the tin impurity) was close to that of the nominal stoichiometric composition. The ingots were powdered and annealed for a long time (up to one month) at the temperatures needed

to obtain an ordered structure. The sample quality was monitored in the course of the annealing by measuring the Mössbauer-absorption spectra for the ^{57}Fe and ^{119}Sn isotopes.

The parameters of the ^{57}Fe spectra, measured at 77 and 295 K, agreed well with the published data. The tin concentration in the alloys was varied in the range from 0.3 to 1.0 at.% for FePd$_3$ and 0.5 to 1.0 at.% for Fe$_3$Pt. In the case of FePt$_3$ the measurements were made only at a tin concentration 1 at.%. The ^{119}Sn spectra were measured with a CaSnO$_3$ γ-ray source at room temperature. The features of the measurement technique and the spectrum reduction procedure are given in our preceding articles.[10,13] We deal below with the results obtained for ^{119}Sn at 77 K.

The ordered alloy FePd$_3$ is a ferromagnet with a Curie temperature $T_c \approx 520$ K. The magnetic moments of the Fe and Pd atoms are respectively 3.1 μ_B and 0.4 μ_B.[14] The absorption spectrum for ^{119}Sn in FePd$_3$ (at a tin concentration 0.3 at.%) is shown in Fig. 1. The form of the spectrum corresponds to one value of H, meaning that the Sn atoms are localized in sites of a single type (only in Fe sites or only in Pd sites). The broadening of the hyperfinestructure components indicates a small spread of the values of H about the mean value ($\Delta H/H \approx 5\%$). This broadening increased with increasing tin content, thus reflecting the high sensitivity of H to the long-range order parameter. Measurements in external magnetic fields have shown that the hyperfine field is positive. Analysis of the spectrum of Fig. 1 has shown that $H = +9.1 \pm 0.2$ T for Sn in FePd$_3$ at 77 K. The measurement error includes the analysis inaccuracies due to the broadening of the hyperfine-structure components.

The alloy Fe$_3$Pt is also a ferromagnet with $T_c = 440$ K. The magnetic moments of the Fe and Pt atoms are respectively 2.8 μ_B and 0.3 μ_B.[15] In this case the hyperfine field for the Sn atoms turned out to be very weak ($H = 0.07 \pm 0.03$ T at 77 K), so that single broadened lines were observed in the spectra. Owing to the weak influence of the MIH on the form of the spectrum, the sign of H was not determined. For Fe$_3$Pt, the dependence of T_c on the long-range order parameter S is well known. This has made it possible to estimate the parameter S for our alloy by determining T_c from the temperature dependences of $H(T)$ for ^{57}Fe and ^{119}Sn. The obtained value $T_c = 435 \pm 2$ K corresponds to $S \approx 0.9$ according to the data of Sasaki and Chikazumi.[16]
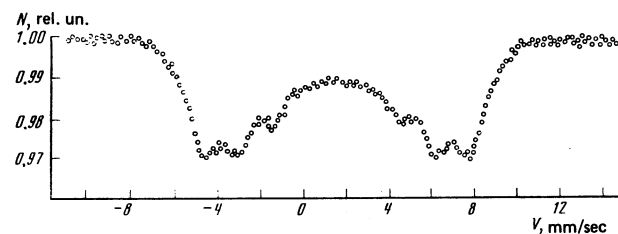
The magnetic structure of the antiferromagnetic al-

loy FePt$_3$($T_N = 190$ K) was investigated by Bacon and Crangle.[17] The magnetic moment of the Fe atom in this alloy is 3.5μ_B, and the moment of the Pt atom is probably zero. The absorption spectrum for ^{119}Sn and FePt$_3$ at 77 K is similar in form to the spectrum in FePd$_e$. The measurements with FePt$_3$ were made only at a high tin concentration (1 at.%), therefore the broadening of the hyperfine-structure components was larger than in FePd$_3$, and corresponded to $\Delta H/H \approx 10\%$. The value of H for the Sn atoms in FePt$_3$ at 77 K was found to be 8.0 ± 0.3 T. When the nonmagnetic impurity atom is localized in a Pt site, the hyperfine field should be zero, since the summary magnetic moments for this site and zero in each coordination sphere. The results show thus that the impurity Sn atoms in ordered FePt$_3$ are localized in the Fe sites. (It will be shown below that the impurity Sn atoms are similarly localized in all three investigated alloys.)

The measurement results will be considered in greater detail in Sec. IV.

III. THE EMPIRICAL FUNCTION $p(r)$ FOR Sn ATOMS IN METALLIC FERROMAGNETS

For Sn atoms in metallic ferromagnets, the MHI can be regarded as isotropic, so that Eq. (1) can be written in the form

$$H = \sum M_i(r_i) p(r_i), \qquad (2)$$

where M_i is the summary magnetic moment of an atom located at a distance r_i from the Sn atom. In the general case, summation over all the coordination spheres is assumed in (2). It is to be expected, however, that at sufficiently large r_i the partial contributions $p(r_i)$ will be negligibly small.

If a universal function $p(r)$ exists for the given type of nonmagnetic atom, then some of its properties can be obtained by comparing the values of H for systems with essentially different radial distributions of the moments M_i. This is possible, of course, if some simplified variant of (2) is used, with a small number of parameters. A similar procedure was used by us earlier[7] to intepret the data for Sn atoms in magnets with bcc structure. A simple empirical formula was obtained, valid for alloys of identical structure and with close lattice constants.

More complete information on the function $p(r)$ can be obtained by generalizing this analysis method, applying it to systems with different structures, and regarding the parameters of the empirical formula as functions of distance. The analysis results become less reliable with increasing number of parameters. We use therefore a simplified variant of (2), stipulating that the number of parameters for each alloy not exceed three. To this end we assume that the summary contribution to H from magnetic atoms located at distances larger than 4 Å can be represented by a single term proportional to the average atomic moment μ of the alloy:

$$H = \sum_{r_i < 4A} M_i(r_i) p(r_i) + C\mu. \qquad (3)$$

N, rel. un.

FIG. 1. Spectrum of Mössbauer resonant absorption for the ^{119}Sn impurity atoms in FePd$_3$ at 77 K.

The coefficient C is assumed to be the same for all the alloys. For all the systems considered below, a sphere of radius 4 Å spans only two coordination spheres, so that for each alloy Eq. (3) is equivalent to

$$H = M_1(r_1)p(r_1) + M_2(r_2)p(r_2) + C\mu, \qquad (4)$$

where the subscripts 1 and 2 number the coordination spheres. The representation of the contribution made to H by atoms located at distances $r > 4$ Å by a single term $C\mu$ is of course a rough approximation, but at the present stage the simplification seems necessary.

The experimental data used to determine the parameters of (4) are given in Table I. The table contains only alloys with the three structure types characteristic of "good" metals (bcc, fcc, hcp). Allowing for the approximate character of (4), we have disregarded the statistical errors in the measurements of H and M_i, and introduced no corrections for the Lorentz field. It was assumed that the distances r_i can be regarded as equal if they differ by not more than 0.03 Å.

We shall show, bcc-structure systems as the example that the values of H are practically independent of the type of atoms making up the alloys, and are determined principally by the relation between the moments M_i and μ. It was shown earlier 7 that for such systems the contributions made to H by the magnetic atoms of the second coordination sphere ($r_2 = 2.85$–3.10 Å) is very small. If we put $p(r_2) = 0$ in (4), we obtain for alloys with close lattice constants [i.e., at $p(r_1) \approx$ const] the simple linear relation

$$H/\mu = (M_1/\mu)p_1 + C. \qquad (5)$$

A comparison of the experimental data (see Table I) with formula (5) is shown in Fig. 2. The very good agreement between (5) and the experimental data confirms the validity of the assumptions made. It is seen that for all the alloys (regardless of their composition) the contribution to H from the second coordination sphere is indeed very small, whereas p_1 is close to -3.0 T/μ_B. Extrapolation of the obtained relation to $M_1 = 0$ yields $C = +20$ T/μ_B. We shall use hereafter this value of the coefficient C to determine the radial de-
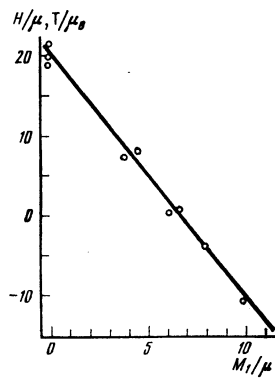

FIG. 2. Linear correlation of H/μ and M_1/μ for Sn atoms in metallic ferromagnets with bcc structure [see formula (5)].

pendence of the partial contributions $p(r_i)$. We note that the choice of the constant C is not completely unambiguous, since a satisfactory description of the data of Table I can be obtained for a certain interval of values of this constant. A change of C is accompanied by a corresponding change of $p(r_i)$, but the shape of the $p(r)$ curve changes insignificantly in this case. We assume that at the present stage the choice $C = +20$ T/μ_B is the most objective.

At a fixed value of the coefficient C, the partial contributions $p(r_i)$ can be obtained by comparing the data of Table I with formula (4). As seen from Table I, for certain alloys only one of the two closest coordination spheres has a nonzero magnetic moment. In such cases, the corresponding partial contribution is determined from (4) directly. In the remaining cases the most probable values of $p(r_i)$ were obtained by a joint analysis of the data for groups of alloys with identical r_i. [For the alloy Fe Al, the value p (2.51 Å) was chosen, close to the value p (2.48 Å) obtained from the data for the matrices of Fe and CoFe.]

The partial contributions $p(r_i)$ obtained in this manner are given in part I of Table II and are shown in Fig. 3. For those cases when $p(r_i)$ was determined from the data for several alloys (as well as for Fe$_3$Al), Table II indicates the possible interval of $p(r)$. We

TABLE I. Magnetic hyperfine fields H for Sn atoms and distribution of magnetic moments M_1 and M_2 in metallic ferromagnets with bcc, fcc, and hcp structures.

Matrix	Site occupied by Sn atom	H, T	r_1, Å	r_2, Å	M_1, μ_B	M_2, μ_B	μ, μ_B
			bcc structure				
Fe	Fe	−8.3 [16]	2.48	2.87	17.6	13.2	2.2
CoFe	Co	−26.0 [7, 19]	2.47	2.85	24.0	11.1	2.42
CoFe	Fe	+0.7 [7]	2.47	2.85	14.8	18.0	2.42
Fe$_3$Al	FeII	+0.8 [7]	2.51	2.90	8.7	9.0	1.30
FeRh	Fe	+14.7 [20]	2.59	2.99	8.0	18.6	2.05
Co$_2$MnSn	Sn	+10.7 [21]	2.59	2.99	6.0	21.5	1.27
Cu$_2$MnSn	Sn	+20.0 [22]	2.67	3.08	0	22.3	0.93
Cu$_2$MnIn	In	+19.6 [23]	2.69	3.10	0	24.0	1.00
Pd$_2$MnSb	Sb	+21.0 [24]	2.78	3.21	0	26.4	1.10
			hfc structure				
Co	Co	−2.3 [25]	2.50	3.54	21.0	10.5	1.75
			hcp structure				
Co	Co	−4.9 [25]	2.50	3.54	20.6	10.3	1.72
Fe$_3$Ge	Ge	−17.4 [10]	2.58	3.65	24.4	0	1.52
Fe$_3$Sn	Sn	−10.3 [26]	2.71	3.83	27.2	0	1.70

TABLE II. Partial contribution to the magnetic hyperfine field for Sn atoms in metallic magnets.

r, Å	$p(r)$, T/μ_B	Matrices
	Part I	
2.48	−3.0±0.10	Fe, CoFe (Fe site), CoFe (Co site)
2.86	−0.1±0.10	
2.51	−2.85±0.05	Fe$_3$Al
2.90	−0.05±0.04	
2.59	−2.1±0.1	FeRh, Fe$_3$Ge
2.99	−0.3±0.2	Co$_2$MnSn
2.71	−1.63	Fe$_3$Sn
3.09	+0.02±0.04	Cu$_2$MnSn, Cu$_2$MnIn
3.21	−0.04	Pd$_2$MnSb
3.54	+2.12±0.15	Co hfc , Co hcp
	Part II	
2.44	−2.95±0.05	Fe$_3$Si
2.77	−0.4±0.1	Au$_2$Mn
3.37	+2.10	
3.74	+0.07±0.15	Fe$_3$Pt
3.84	−0.23	FePd$_3$

Note. The data listed in parts I and II of the table are dealt with in Sec. III and IV of the article, respectively.

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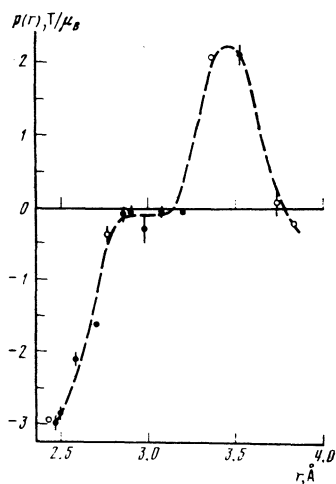
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FIG. 3. Empirical function $p(r)$ of the radial dependence of the partial contributions for the Sn atoms in metallic magnets. The dark and light circles show the data listed in parts I and II, respectively.

note that Table I lists data only for those alloys in which the localization of the Sn atom has been reliably determined. In the next section of the article we consider other data and obtain additional information on the partial contribution (part II of Table II).

It is important that the $p(r)$ curve that can be drawn through the obtained values of $p(r_i)$ be smooth enough and that the values of $p(r_i)$ for close r_i agree well with one another. Characteristic features of the obtained $p(r)$ dependences are a strong radial dependence of the negative partial contribution in the region $r = 2.5-2.8$ Å, a reversal of the sign at $r \approx 2.9-3.2$ Å, and a large positive maximum at $r \approx 3.5$ Å. These qualitative features of the function $p(r)$ follow directly from the systematics of the experimental data and do not depend on the approximations made. At the same time, the concrete values of $p(r_i)$ must be regarded as approximate, with an accuracy that depends both on the degree to which (4) is approximate and on the accuracy of the choice of the constant C. Nonetheless, the obtained variant of the function $p(r)$ is sufficient for a consistent interpretation of a large number of experimental data, a fact that should be regarded as a confirmation of the relative independence of the function $p(r)$ of the composition and structure of the alloys.

It would be interesting to compare the function $p(r)$ obtained for the Sn atoms with the analogous data for other atoms. One should expect the form of $p(r)$ to depend on the atomic number of the element; this dependence might be an important criterion for the choice of an adequate MHI model. Unfortunately, the possibilities of such a comparison are extremely limited. We have so far no concrete data on the radial dependence of the partial contributions in the case of other nonmagnetic atoms. Stearns[3,6] performed direct measurements for Fe atoms in alloys with bcc structure. (The Fe atoms have a magnetic moment, but Stearns' data pertain to that part of H which is determined by the magnetic surrounding.) According to the

Stearns model,[3] the "volume contribution" to H, due to the overlap of the electron functions, is zero for Fe atoms, whereas for Sn atoms this contribution is comparable with the contribution of the contact interaction with the conduction electrons. It is to be expected therefore that the functions $p(r)$ for the atoms Fe and Sn differ greatly (at least for short distances).

What is noteworthy in the comparison of the obtained data is not so much the difference as the expected similarity of the $p(r_i)$ dependences for two types of atoms. Just as for the Sn atoms, the partial contributions for the Fe atoms are large and negative at $r \approx 2.5$ Å, and decrease in absolute value with increasing r. At $r \approx 3$ Å the function $p(r)$ reverses sign and becomes positive. A positive maximum of $p(r)$ is observed at approximately the same value of r as for the Sn atoms. The most substantial difference lies in the relative weights of the partial contributions of opposite sign: for the Sn atoms, in most cases, the positive and negative components of H are comparable, whereas for the Fe atoms the negative contribution from the nearest neighbors always predominates. The Stearns data were obtained only for systems with one type of structure and close lattice constants, so that the detailed behavior of $p(r)$ in the distance range 2.5–4.0 Å is unknown. Nonetheless, the great similarity of the $p(r)$ functions for the Fe and Sn atoms is undisputed, so that it is of particular interest to obtain analogous data for other atoms.

The $p(r)$ dependence obtained for Sn atoms can be compared with RDSD calculations based on the d-resonance theory.[5] Some properties of $p(r)$ [the large negative $p(r_i)$ at $r = 2.5-2.7$ Å, the reversal of sign at $r = 2.8-3.0$ Å, and the positive maximum at $r \approx 3.5$ Å] can be confirmed by the RDSD curve at the wave-vector value $k_F \approx 1.5 \times 10^8$ cm^{-1}. This comparison, however, is only purely illustrative, since the choice of k_F is arbitrary. In addition, within the framework of the d-resonance theory it is difficult to explain the very existence of a "universal" function $p(r)$, i.e., the relative independence of this function of the composition and structure of the alloys.

IV. USE OF THE EMPIRICAL FUNCTION $p(r)$ FOR THE INTERPRETATION OF CERTAIN EXPERIMENTAL DATA

The obtained empirical function $p(r)$ can be used to interpret other data on the MHI for impurity Sn atoms in metallic magnets. We shall show that the obtained information on the radial dependence of $p(r)$ is sufficient in a number of cases for an unambiguous determination of the localization of the impurity atom in the lattice site. We shall obtain simultaneously new data on the radial dependences of the partial contributions.

1. $FePd_3$, Fe_3Pt. According to the results considered in Sec. II, the values of H for the Sn impurity atoms in these ferromagnetic matrices with fcc structure are respectively $+9.1$ and 0.07 T. At $C = 20$ T/μ_B formula (4) takes for these cases the form

$$H = M_1 p(2.71) + M_2 p(3.84) + 21.6 \quad (\text{FePd}_3),$$

$$H = M_1 p(2.64) + M_2 p(3.74) + 43.5 \quad (\text{Fe}_3\text{Pt}). \tag{6}$$

Here and below the numbers in the parentheses following p are the distances in Å. The moments M_i and the partial contributions $p(r_i)$ are given below in units of μ_B and T/μ_B, respectively.

The previosuly obtained data (see the first part of Table II and Fig. 3) allows us to regard $p(r_1)$ as known: we assume $p(2.64) = -1.95 \pm 0.05$ and $p(2.71) = -1.63$. It is easily seen that the assumption that the Sn atoms are localized in the Pd(PT) sites leads to a patent disparity with experiment. In this case ($M_1 = 1.56, M_2 = 2.4$ in FePd$_3$, $M_1 = 33.6, M_2 = 1.8$ in Fe$_3$Pt) we obtain for all reasonable values of $p(r_2)$ a small negative or close-to-zero H in FePd$_3$ and a large negative H in Fe$_3$Pt. At the same time the assumption that the Sn atoms are localized in the Fe sites leads to a consistent interpretation of the experimental data. In this case $M_1 = 5.0$, $M_2 = 18.6$ in FePd$_3$ and $M_1 = 23.6$, $M_2 = 16.8$ in Fe$_3$Pt. Since the $p(r_1)$ are known, we find from (6) that $p(3.74) = +0.07 \pm 0.15$ and $p(3.84) = -0.23$. These values are in good agreement and point to the existence of a second node of the function $p(r)$ at $r \approx 3.8$ Å (Fig. 3).

2. Au$_2$Mn. For Sn impurity atoms in the helimagnet Au$_2$Mn, two values of H were obtained, $H_1 = 6.0$ T and $H_2 = 30.2$ T.[27] It was suggested[27] that H_1 and H_2 correspond to Sn atoms localized in the Mn and Au sites, respectively.

The data obtained in the present study of the radial dependence of $p(r)$ force use to accept the opposite interpretation. In fact, for the two posssible localizations of the Sn atoms in Au$_2$Mn, formula (4) takes the form

$$H = 14.4\, p(3.37) \quad (\text{site Mn}), \tag{7a}$$

$$H = 14.4\, p(2.77) + 2.9\, p(3.0) \quad (\text{site Au}). \tag{7b}$$

Equation (7a) makes it possible to determine $p(3.37)$ directly for a given H. The value of $p(3.0)$ is already known, and from (7b) we can ontain $p(2.77)$, which should be close to -0.5 according to the data of Fig. 3. This leads to the unambiguous conclusion that $H_1 = 6.0$ T corresponds to Sn atoms in Au sites, while $H_2 = 30.2$ T corresponds to Sn atoms in Mn sites. In this variant [at $p(3.0) = -0.3 \pm 0.2$] we obtain $p(2.77) = -0.4 \pm 0.1$ and $p(3.37) = 2.1$, in good agreement with the proposed form of the function $p(r)$ (Fig. 3).

3. Fe$_3$Si. For the impurity Sn atoms in the bcc-structure ferromagnet Fe$_3$Si the field $H = -5.0$ T.[7] In this case the Sn atoms can be localized in sites of three types: FeI, FeII, and Si. The expression for H contains the partial contributions $p(2.44)$ and $p(2.82)$, the first of which should not differ greatly from the already known $p(2.48)$, while the second should be close to -0.15. The specific character of the M_i distribution does not allow an unambiguous localization of the Sn atoms. An equally good agreement with experiment is obtained for the sites FeI and FeII at $p(2.44) = -2.95 \pm 0.05$. This value of $p(2.44)$ is in good agreement with $p(2.48) = -3.0 \pm 0.1$.

4. *Antiferromagnetic matrices.* The approximation

based on formula (4) may turn out to be particularly rough for antiferromagnets, for in this case $\mu = 0$ and the contribution made to H by the atoms outside a sphere of radius 4 Å is not taken into account at all. Nonetheless, calculation by formula (4) for the Cr matrix agrees well with experiment. For Sn atoms in antiferromagnetic Cr formula (4) takes the form

$$H = 3.4\, p(2.50) - 2.5\, p(2.88),$$

with both partial contributions already known. At $p(2.50) = -2.9$ and $p(2.88) = -0.1$ we get $H = -9.6$ T, in splendid agreement with the measured $H = \pm 9.8$ T.[28] (The minus sign means in this case that the magnetic field is antiparallel to the magnetic moment of the first coordination sphere.)

In much worse agreement with the obtained $p(r)$ dependence are the data for impurity Sn atoms in the antiferromagnetic matrices of γ-Mn (Ref. 29) and FePt$_3$. To explain these data within the framework of the approximation based on (4) we need partial contributions $p(3.86) \approx p(3.86) \approx +1.0$, substantially different from the $p(3.84) = -0.23$ obtained for the ferromagnetic FePd$_3$ matrix.

All the data obtained in this and preceding sections on the partial contributions $p(r_i)$ are shown in Fig. 3 and Table II. The possibility of a consistent interpretation of the data for a large group of metallic magnetic matrices can be regarded as an undisputed success of the empirical method of determining the function $p(r)$. It must be pointed out at the sime time that among the experimental data on MHI for Sm atoms there are at least three cases that contradict the general mass to one degree or another.

A known example of such an "anomaly" is the ferromagnetic Geissler alloy Pd$_2$MnSn. The Pd in this alloy are nonmagnetic, so that from the point of view of the distribution of the moments M_i this alloy is equivalent to the alloys Cu$_2$MnSn, Cu$_2$MnIn and Pd$_2$MnSb listed in Table I. However, whereas the values of H for the Sn atoms in these three alloys are practically the same and close to $+20$ T, a weak negative field $H = -3.5$ T is observed in Pd$_2$MnSn.[22] There are no data whatever to indicate some special properties of Pd$_2$MnSn compared with other alloys with analogous composition. It is therefore difficult to propose a reasonable explanation of the anomalous value of H for Sn atoms in Pd$_2$MnSn.

The ordered Ni$_2$MnSn is also a ferromagnet Geissler alloy. If (as proposed) the magnetic moment of the Ni atoms in this alloys is zero, then H for the Sn atoms should be close to $+20$ T (as for the three other alloys mentioned above). The measured value of H, however, is approximately half as large, $H = +8.7$ T.[22] It cannot be ruled out that this "anomaly" is caused by the fact that the real moment of the Ni atom is not zero. To reconcile the measured value of H with the empirical function $p(r)$ it suffices to assume that the magnetic moment of the Ni atom is close to 0.6 μ_B.

For Sn atoms in the ferromagnetic alloy Co$_2$TiSn, the empirical function $p(r)$ corresponds to $H \approx -6$ T, as against the measured $H = +8.5$ T.[30] It is possible that

in this case we have an example of a ferromagnetic system for which the approximation based on (4) is too rough. Only the Co atoms in this alloy have a magnetic moment, therefore the magnetic polarization spheres are far from one another ($r_1 = 2.63$ Å, $r_2 = 5.03$ Å). Replacement of the real distribution of the moment M_i at $r > 4$ Å by the average moment μ can lead in this case to a substantial decrease of the positive contribution to H, especially if, for example, the function $p(r)$ has a second positive maximum at $r \approx 5$ Å.

It must be emphasized that the regularities considered above and the empirical function $p(r)$ correspond to MHI for Sn atoms only in metallic magnets, i.e., in systems with a definite type of intereaction between the atoms. The selection criteria of these systems are not rigorously defined, and we have therefore confined ourselves to consideration of the data for alloys with the three types of structures that correspond most closely to good metals. For intermetallides with more complicated structures (where, e.g., covalent interaction between atoms is significant), the form of the function $p(r)$ can be entirely different.

Further experiments will make it possible to refine the functions $p(r)$ and the applicability limits of the assumptions made, but the most important task should be the finding of analogous data on the function $p(r)$ for other nonmagnetic atoms. We propose that an investigation of the dependence of the type of the function $p(r)$ on the type of the atom is at present the best (if not the only) method of choosing an adequate MHI model for nonmagnetic atoms in metallic magnets.

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