Muon hyperfine fields in Fe(Al) alloys

C. E. Stronach*
Virginia State University, Petersburg, Virginia 23803

W. J. Kossler, J. Lindemuth,† and K. G. Petzinger
The College of William and Mary, Williamsburg, Virginia 23186

A. T. Fiory and R. P. Minnich
Bell Laboratories, Murray Hill, New Jersey 07974

W. F. Lankford
George Mason University, Fairfax, Virginia 22030

J. J. Singh
NASA Langley Research Center, Hampton, Virginia 23665

K. G. Lynn
Brookhaven National Laboratory, Upton, New York 11973
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The hyperfine field on the muon, B_{hf}, at interstitial sites in dilute Fe(Al) alloys has been measured for four different concentrations of Al and as a function of temperature by the muon-spin-rotation method. The magnitude of B_{hf}, which is negative, decreases at rates ranging from $(0.09 \pm 0.03)\%$ per at.% Al at 200 K to an asymptotic limit of 0.35 ± 0.03 far above 440 K. This behavior shows that sites near the Al impurity are weakly repulsive to the muon, with an interaction potential of 13 ± 3 meV. In order to fit the temperature dependence of the hyperfine field, it is necessary to hypothesize the existence of a small concentration of unidentified defects, possibly dislocations, which are attractive to the muon. Although the Al impurity acts as a nonmagnetic hole in the Fe lattice, the observed decrease in B_{hf} is only 35% of the decrease in the bulk magnetization. We conclude that B_{hf} is determined mainly by the enhanced screening of conduction electrons in Fe and Fe(Al). Since the influence of the Al impurity on the neighboring Fe moments is very small, most of the change in B_{hf} is therefore attributed to the increase in conduction-electron polarization at the Al impurity.

I. INTRODUCTION

Knowledge of the local electronic structure around the isotopes of hydrogen, when present as impurities in metal and alloys, is fundamental to a basic understanding of the diffusion of these particles and their poorly understood interaction with defects and impurities, particularly in Fe. Measurements of the Fermi contact or hyperfine field on positive muons can help provide this information.[1-3] We have studied Fe(Al) alloys with muon-spin-rotation methods (μSR) to help formulate a physical picture of the local magnetic field and how the host electrons participate in screening the muon's positive charge. Information is also obtained on the mutual interaction between the positive muon and the Al impurities in the Fe host.

The muon probes the magnetic fields at interstitial sites, so that it is specifically sensitive to the extent to which electron states in metals are delocalized, or bandlike. As an example of how this is accomplished, we refer to the recent work of Hayano *et al.* who have compared μSR and host NMR measurements in a study of the itinerant magnetism of the helimagnet MnSi.[4] General applicability of this aspect of such measurements is of course contingent on being able to correctly account for the perturbation which the muon creates in the metal. The problem appears to be tractable and several theoretical approaches have been advanced.[1-3,5] The pure elemental ferromagnets Ni,[6-10] Fe,[6,7,9-12] Co,[7,9,13,14] Gd,[15,16] and Dy[17] have been among the metals studied with muons.

The basic properties of the muon in metals may be derived from the assumption that the *s*-like conduction-band electrons are mainly responsible for screening the muon's charge. This interpretation has been proposed for the case of Ni,[1,2] assuming *d*-like states contribute very weakly to the screening at the muon site, even though there is a high density of *d* states at the Fermi level. However, the *s*-like bands

of Ni have little or no polarization, and the muon therefore experiences a negative hyperfine field which is dominated by the tails of the minority-spin *d*-like wave functions in the interstitial region. The theoretical basis for this model was discussed by Petzinger and Munjal[1] and by Petzinger.[2] This model takes the opposite view to what had been previously supposed for hydrogen in transition metals.[18] Patterson and Keller[5] recently carried out a finite cluster calculation which lends additional support to this model, in that the *d* electrons remain on the neighboring Ni atoms in the cluster.

The above model is thought to be applicable to Fe in spite of the more complicated band structure, where more significant *s*-*d* hybridization is found.[19] Jena has discussed the nonlinear screening of the muon in Fe in terms of a free-electron gas,[3] where the ambient spin density is increased by a factor of 9.8. The measured hyperfine field on the muon is -11 kG, so that on applying this model one finds that the ambient polarization density is effectively $-0.014\,\mu_B$ Å^{-3}. By comparison, neutron-diffraction measurements[20] give a value of $(-0.014 \pm 0.004)\,\mu_B$ Å^{-3}, averaged over a 0.5-Å cube centered at the tetrahedral interstitial site where the muon is presumed to reside.[21] The neutron data also show that there is a delocalized background polarization of $-0.21\,\mu_B$ per atom, which is equivalent to a homogeneous polarization density of $-0.018\,\mu_B$ Å^{-3}.[20] This indicates that the muon hyperfine field is obtained following two quite different assumptions, that the muon experiences either the average conduction-electron polarization or the local polarization at a particular site. Band-structure calculations have found that the 4*s*-electron contribution to the polarization is between -0.04 and -0.07 μ_B per atom.[19] This does not include the contribution from itinerant *d* states, which is apparently larger. Thus, our view is that previous work indicates that itinerant states in Fe might be treated as a free-electron gas in screening the muon.

Alloys of various nontransition elements in Fe have been studied by bulk-magnetization measurements,[22,23] neutron diffraction,[24,25] NMR,[26–29] and the Mössbauer effect.[29–31] These measurements found that the Al impurity produces simple magnetic dilution. Neutron-diffraction studies have confirmed that the Al is nonmagnetic and that the surrounding Fe neighbors exhibit very little perturbation on their moments. The NMR and Mössbauer satellite lines have been associated with Al in various neighbor shells around the Fe. Grüner *et al.*[29] have shown that these results can be explained by the spin-polarized conduction-electron cloud around the Al. More recently, Terakura has proposed a theoretical explanation based on an *ab initio* calculation of the electronic densities and polarizations at the Al site.[32] He found a net increase in the *s*-*p* polarization at the Al site. His predictions for Si impurities are quite similar to those for Al.

This paper is an elaboration and an extension of our previous studies of Fe(Al) with muons.[33] Additional studies of ferromagnetic alloys were recently reported by Kossler *et al.*[34] for Ni(Co) and Ni(Cu) and by Nishida *et al.*[35] for Ni(Cr), Fe(Si), and Fe(Ti).

II. EXPERIMENT

μSR is a perturbed angular distribution technique and it has been discussed extensively in the literature.[6,36,37] Spin-polarized positive muons are implanted into the sample under investigation and the time intervals for individual positron decays are recorded. The anisotropy of the positron decay and the precession of the muon spin in the local magnetic field give rise to an oscillatory component in the time dependence of the measured positron emission rate in a given direction. The present studies were done at zero external magnetic field on the samples and used positron detectors at 0° and 180° with respect to the μ^+ beam. The time distribution of the positrons is given by the following formula:

$$N_{e^+}(t) = N_0 \exp(-t/\tau_\mu)[1 + a + b\exp(-\lambda t) \times \cos(\omega t + \phi)] + N_{\text{back}} \quad . \quad (1)$$

N_0 is an overall normalization, τ_μ is the muon lifetime of 2.2 μsec, λ is the depolarization rate, ω is the spin-precession angular frequency, and ϕ is a geometrical phase, essentially the angular coordinate of the positron detector. The values of a and b depend upon the distribution of the orientations of the local fields in the sample and upon the angle subtended by the detector.[37] Taking the case of an unmagnetized ferromagnetic sample, where the local fields are isotropically distributed, and longitudinal placement of the detector, we have $a = \frac{1}{3}P$ and $b = \frac{2}{3}P$, where P is a function of the polarization of the muon beam and the energy dependence of the positron detection efficiency.[37] For our experiment $P \approx 0.1$. The term N_{back} is included to account for accidental background counts in the data.

The experiments were performed at temperatures ranging from 80 to 433 K. The data were fitted with Eq. (1) using a multiparameter least-squares fitting routine. We did not attempt to find the term proportional to a, but rather include it into the definition of N_0 and b in fitting the data. The field on the muon is given by $B_\mu = \omega\gamma_\mu^{-1}$ where $\gamma_\mu = 8.51 \times 10^4\,\text{sec}^{-1}\,\text{G}^{-1}$.

Four spherical samples were fabricated, one of 99.99%-pure Fe, the others containing 1.60, 4.29, and 5.81 at.% Al. The sample materials were melted in a MgO crucible in a He atmosphere by rf induction. The Al was added by including Fe(Al) alloy in the

TABLE I. Properties of the Fe(Al) spheres used in this study. The impurity concentrations measured by atomic absorption analysis for Al, by vacuum fusion analysis for C, O, and N, and by mass-spectrographic analysis for the other elements are given in atomic per cent under the element headings. He and H were below the limits of detectability, 0.0001% and 0.0005%, respectively. An additional estimated 0.2-at.% Al is present in sphere No. 3 in the form of Al_2O_3 precipitates.

No.	Mass (g)	Al	C	O	N	Si	Ni	Zr	Ti	Mg	Cu
1	766.91	0.001	0.002	0.64	0.003	0.004	0.005	0.003	0.0005	0.0005	0.0002
2	760.84	1.60	0.002	0.01	0.003	0.008	0.005	0.003	0.0005	0.0005	0.0002
3	743.22	4.29	0.013	0.3	0.01	0.008	0.005	0.003	0.0005	0.0005	0.0002
4	739.88	5.81	0.002	0.01	0.003	0.008	0.005	0.003	0.0005	0.0005	0.0002

melt. The melt was poured into an Al_2O_3-coated Fe mold and allowed to cool in the furnace. The castings were 6 cm in diameter and 20 cm in length. Each casting was reheated to 1273 K and hot pressed, reducing the length by a factor of 2. This is a standard procedure for removing most of the casting structure in Fe and its alloys. The castings were then machined to 5.715 ± 0.001-cm-diameter spheres and annealed in H_2 at 1088 K for one hour. At the concentrations used here, the Al is in a random solid solution.[38] The results of a chemical analysis on the samples is given in Table I. After the μSR runs, the spheres were sectioned for analysis. The sizes of the macroscopic crystallites vary between 0.1 and several mm. The 4.29%-Al sample contains, in addition, dispersed Al_2O_3 precipitates on the order of 1 μm across, which accounts for the high oxygen concentration in the analysis (there is a thermite reaction between aluminum and oxygen). From transmission electron microscopy, the dislocation density is on the order of 10^8 cm^{-2} and the subgrain cells are about 1 μm across.

III. DATA ANALYSIS

A. Extraction of the hyperfine field

The results for the magnetic fields on the muon and the depolarization rates are listed in Table II. Values of B_μ given in brackets were obtained by linearly interpolating the temperature dependence of the results on pure Fe given by Nishida *et al.*[11] The hyperfine fields were extracted in the following manner.

The field experienced by the muon may be decomposed[39] into

$$B_\mu = B_{\text{ext}} - B_{\text{dm}} + B_L + B_{\text{dip}} + B_{\text{hf}} \ , \tag{2}$$

where B_{ext} is the applied external field, B_{dm} is the demagnetizing field which depends upon sample geometry, B_L is the Lorentz cavity field $4\pi M/3$ where M is the domain magnetization, B_{dip} is the sum of the dipole fields inside the Lorentz sphere, and B_{hf} is the Fermi contact or hyperfine field. Because we performed the experiment with zero external field, and since the μ^+ particles hop rapidly from site to site, averaging B_{dip} to zero, the expression for B_{hf} reduces to

$$B_{\text{hf}} = B_\mu - B_L \ . \tag{3}$$

The temperature dependence of the Lorentz cavity field was computed following the parameterization of magnetization data for pure Fe given by Redi[40]:

$$M = M_0 f(T) = M_0[1 - A(T/T_C)^{3/2} - B(T/T_C)^{7/2}] \ , \tag{4}$$

where $A = 0.102 \pm 0.005$, $B = 0.33 \pm 0.07$, and $M_0 = 1749$ G. We have assumed that the temperature dependence scales with the Curie temperature of the alloy, given as[41]

$$T_C = T_{C0}(1 - 0.1c) \ , \tag{5}$$

where $T_{C0} = 1044$ K is the Curie temperature of pure Fe and c is the Al concentration. The magnetization is also corrected for the presence of Al in the sample by summing the effects of simple dilution, i.e., replacing Fe atoms with Al atoms and taking into account the known change in lattice spacing.[42] The change in lattice spacing Δa_0 gives a density factor $3\Delta a_0/a_0$, which becomes $0.157c$. Combining these factors yields

$$B_L = \frac{4\pi M}{3}(1 - 1.157c) \ , \tag{6}$$

with M given by Eq. (4).

The resulting values of B_{hf} are listed in Table II. The data for sphere No. 1 are consistent with pure Fe data of Nishida *et al.*[11] The data and fit for B_{hf} at 301 K as a function of concentration are plotted in Fig. 1. The change in B_{hf} is (-0.234 ± 0.004)% per at.% impurity at 301 K.

The reduced quantity $\Delta B_{\text{hf}}/cB_{\text{hf}}$ for $c = 0.0429$ is plotted as a function of temperature in Fig. 2. Muon precession oscillations were observed only at 200 K

TABLE II. Observed magnetic fields on the muon B_μ, muon-spin depolarization rates λ, calculated Lorentz cavity fields B_L, and resultant Fermi-contact hyperfine fields B_{hf}. Errors of measurement are enclosed in parenthesis. Values of B_μ enclosed in brackets were interpolated from the data of Nishida *et al.* (Ref. 11). c is the Al impurity concentration in atomic per cent.

c	T (K)	B_μ (G)	λ (μsec^{-1})	B_L (G)	B_{hf} (G)
0	200	[−3672(2)]		7256	−10928
	240	[−3638(2)]		7230	−10868
	260	[−3621(2)]		7215	−10836
	280	[−3604(2)]		7198	−10802
	301	[−3590(1)]		7179	−10769
	301	−3592(3)	3.0(3)	7179	−10771
	343	[−3530(4)]		7136	−10666
	373	−3477(2)	2.2(2)	7101	−10578
	433	−3379(3)	1.5(1)	7016	−10394
1.60	301	−3687(2)	1.4(2)	7046	−10733
4.29	200	−3990(14)	9(2)	6896	−10886
	240	−3954(5)	3.8(4)	6870	−10824
	260	−3902(2)	2.9(2)	6856	−10758
	280	−3866(2)	2.0(1)	6840	−10706
	301	−3842(2)	1.7(3)	6822	−10664
	343	−3772(1)	1.5(1)	6781	−10553
	373	−3719(1)	1.0(1)	6746	−10466
	433	−3612(1)	1.0(1)	6665	−10277
5.81	301	−3930(2)	1.3(2)	6695	−10625

and above, presumably because the muons are trapped at defects below about 200 K. It is seen that the fractional change in hyperfine field is temperature dependent.

B. Temperature dependence of B_{hf}

The temperature dependence of the change in B_{hf} with Al concentration (Fig.2) can be explained if the diffusing muons do not randomly sample the interstitial sites in the alloy. This does not invalidate the assumption that B_{dip} averages to zero because the preference in sampling relates to the presence of an Al nearest neighbor rather than to the two magnetically inequivalent tetrahedral interstitial sites. In general, the average hyperfine field is obtained by summing local contributions from all available sites, weighted according to Boltzmann population factors;

$$B_{hf} = \sum_i B_{hf}^i \exp(-\beta E^i)/Z \quad , \tag{7}$$

where $\beta = (kT)^{-1}$, E^i is the state energy of the muon at sites i, B_{hf}^i is the local hyperfine field at sites i, and Z is the thermodynamic partition function.

In order to give this effect a quantitative treatment, we consider the following model. First, we assume that the E^i vary significantly only at sites immediately adjacent to impurities and defects. Second, we assume that the muon energy is changed by an amount E' for a fraction c' of sites which are near the Al impurity. Defects are taken into account by including a fraction c'' of sites with energy E'' relative to the unperturbed sites. Since there are 24 tetrahedral inter-

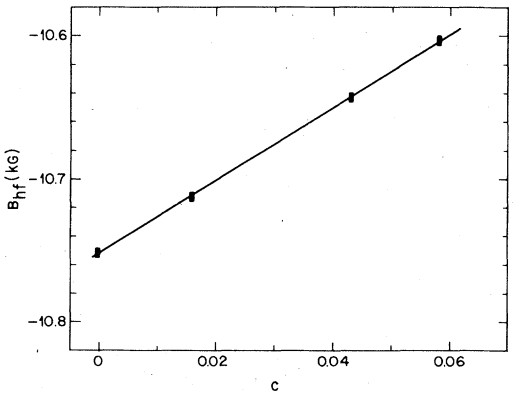

FIG. 1. Fermi-contact hyperfine field on the positive muon in Fe(Al) as a function of impurity concentration at a temperature of 301 K. The line is a least-squares fit.

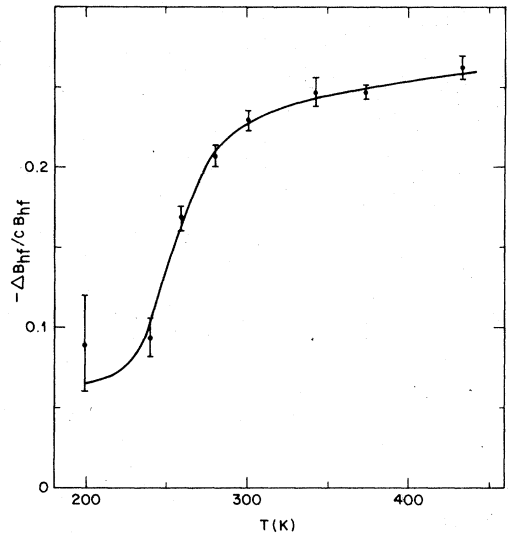

FIG. 2. Temperature dependence of the fractional change in the hyperfine field with aluminum concentration. Data were taken for $c = 0.0429$. The curve is the fitted function Eq. (8) divided by c, using the parameters of Table III.

stitial sites around each Al atom, as opposed to the six tetrahedral sites per Fe atom, we take $c' = 4c$, for consistency. If we write the field near the Al sites as B'_{hf}, the field at the defect sites B''_{hf}, and the field elsewhere as B^0_{hf}, then the average hyperfine field is given by

$$\frac{\Delta B_{hf}}{B^0_{hf}} = \frac{f'c'\exp(-\beta E') + f''c''\exp(-\beta E'')}{1 - c' - c'' + c'\exp(-\beta E') + c''\exp(-\beta E'')} , \tag{8}$$

where we have used the reduced parameters

$$f' = 1 - B'_{hf}/B^0_{hf}$$

and

$$f'' = 1 - B''_{hf}/B^0_{hf} .$$

The data of Fig. 2 were fitted with Eq. (8) by treating f', f'', c'', E', and E'' as adjustable parameters. The results are listed in Table III.

TABLE III. Parameters fitting Eq. (8) to the temperature dependence of the hyperfine field in the 4.29-at.% Fe(Al) alloy. f' and f'' are the fractional changes in the hyperfine field, c' and c'' are the site concentrations, E' and E'' are the site energies, for Al and defect sites, respectively. The parameter $c' = 4c$ was held constant.

f'	−0.087(7)
f''	−0.0032(8)
c'	0.172
c''	$10^{-11.7 \pm 3.6}$
E'	0.013(3) eV
E''	−0.6(2) eV

We find that the rapid dependence of $\Delta B_{hf}/cB_{hf}$ near 250 K, followed by a comparatively gentle dependence at higher temperatures, can therefore easily be explained in terms of a small concentration of strongly attractive defect sites and weakly repulsive Al sites. The reduced χ^2, for three degrees of freedom, is 0.54 for the fit given in Table III. For comparison, we also tested an alternative fit to the data by omitting the defect term, i.e., with $c'' = 0$. The asymptotic value of $\Delta B_{hf}/cB_{hf}$ turns out to be 40% larger and E' a factor of 2 larger. However, the reduced χ^2, for six degrees of freedom, increases to 10. The statistical probability that the defect term gives a better fit is therefore 0.99.

The asymptotic value of B_{hf}/cB_{hf} approaches -0.35 ± 0.03 at very high temperatures (it is −0.31 at the Curie point, 1043 K), and we take this to be the average hyperfine-field shift for random sampling by the muon. The hyperfine field on the muon at sites near Al is weaker by $8 \pm 1\%$ with respect to pure Fe. The three parameters characterizing the defect sites might be determined better if we had more data in the low-temperature region. We therefore regard these values as approximate. From the small value of the defect concentration found in the fit, $c'' \simeq 10^{-9}$, it seems that dislocations and subgrain boundaries would be the likely explanation. Our result does, however, indicate that the shift in the hyperfine field with impurity doping can be developed as a technique for studying the muon-impurity interaction. It could be complementary to depolarization measurements which study the motional narrowing effect of muon motion.[9–12] These points are discussed further in Secs. III C and IV.

C. Depolarization rates

The μSR signal is observable in Fe and Fe(Al) when the rapid motion of the muon nearly averages out the dipolar field. From the depolarization rate the correlation time of the local dipolar field on the muon can be calculated, and this is nearly the same as the mean time of stay at an interstitial site. The second moment of the dipolar field distribution is about $\langle(\Delta B_{dip})^2\rangle = (2.6\ \text{kG})^2$, owing to the existence of two magnetically inequivalent tetrahedral sites in pure Fe.[11] The value is nearly the same for the Fe(Al) alloy, although the spatial distribution differs. The depolarization rate measured at 301 K for our samples is about a factor of 10 larger than those measured in high-purity Fe,[12] and does not appear to be very sensitive to the Al concentration. Since samples of Fe of nominally lesser purity typically show larger depolarization rates, this effect has been attributed to longer mean times of stay for muons at sites near or at defects. We could assume, therefore, that

the diffusing muons spend part of their lifetime sampling some kind of defect sites throughout the temperature range covered. Clues as to the nature of these defects are obtained by comparing the hyperfine-field shift and depolarization data. The fact that the depolarization in the alloys is weaker than for our pure Fe may be due to the scavenging of impurities such as oxygen and nitrogen by the aluminum.

The depolarization measurements for the 4.29-at.% alloy given in Table II show a monotonic decrease with temperature, with a tendency towards saturation at high temperatures. Thus it appears that the mean time of stay decreases steadily with temperature and that there is a background contribution to the depolarization rate. We consider expressing these data as follows:

$$\lambda = \gamma_\mu^2 \langle (\Delta B_{\rm dip})^2 \rangle f^2(T) \tau_c + \gamma_\mu \Delta B f(T) \quad . \tag{9}$$

The first term represents the motionally-narrowed local dipolar inhomogeneity and the second term the macroscopic magnetization inhomogeneities. τ_c is a correlation time, which we assume has an Arrhenius temperature dependence;

$$\tau_c = \tau_0 \exp(U/kT) \quad . \tag{10}$$

The function $f(T)$ is the same as that given in Eq. (4) and it is included in Eq. (9) in order to correct for the temperature dependence of the dipolar fields. The data do not show any evidence for diffusion limited capture by deep traps (no detrapping), which would have a τ_c^{-1} dependence.[12,43] A trapping term had been considered by Kossler *et al.*[43] in their interpretation of the non-Arrhenius temperature dependence of the depolarization rate in Cr and by Nishida *et al.*[12] in a study of Fe.

The results of a nonlinear least-squares fit of Eqs. (9) and (10) to the depolarization data yields the Arrhenius plot of the correlation time given in Fig. 3. The parameters of the fit are $\Delta B = 8.8 \pm 0.2$ G, $\tau_0 = 0.3$ ps, and $U = 0.11 \pm 0.02$ eV. The statistical uncertainty in τ_0 is about a factor of 10.

We note that the activation energy U for the muon jump processes is about a factor of 4 smaller than the magnitude of the defect interaction energy E'' (see Table III) found in the fit of the hyperfine-field shift. This difference needs explanation. One consistency check concerns whether the muon jump rate is high enough for the muons to reach the defects. A fair test can be made at $T = 250$ K, where the change in the hyperfine field with temperature is most rapid. At this temperature $c'' \exp(-\beta E'') \approx 1$, with muons spending about one-half their time at the defect sites, according to our previous analysis. It can be readily estimated that over the mean duration of the measurement, which is $\lambda^{-1} \approx 0.3$ μsec at 250 K, the muon executes $N \approx \lambda^{-1} \tau^{-1}$ jumps, where τ is jump time. A possible value for τ is 5 ps, obtained by

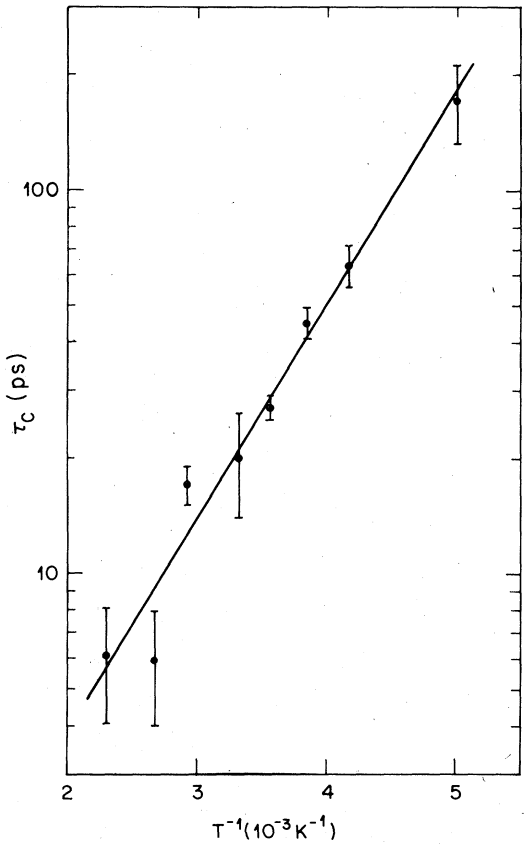

FIG. 3. Dependence of the local-field correlation time upon inverse temperature, obtained from depolarization rates according to Eqs. (9) and (10). The curve is the fitted function.

Nishida *et al.*[12] for high-purity Fe at 250 K, with the result $N \approx 6 \times 10^4$. Equilibrium sampling of defects would be approached when $Nc'' \approx 1$. On the contrary, we find $Nc'' < 10^{-4}$. To resolve the apparent discrepancy we propose the following: (a) The defects are dislocations and subgrain boundaries, whose effective site concentration is very small; (b) E'' is some average muon-dislocation binding energy; (c) the muons are mobile along the dislocations, with an activation energy of migration U; and (d) the muon mean time of stay at unperturbed interstitial sites in Fe is probably much smaller than 5 ps at 250 K.

IV. DISCUSSION

A simple view of the effect of dilute Al impurities is first that the Al is substitutional in Fe and the contribution from the d states of the removed atom can be simply subtracted. Invoking the observation that the moments of the Fe atoms are nearly unperturbed, we then assume that the d-electron contribution to the average hyperfine field on the muon is

simply decreased by 1% per at.% Al. Further support for this assumption comes from the fact that the magnetic disturbance has only a weak dependence on the valence of the impurity atom.[24,25] There is a similarly small perturbation on the neighboring Fe for Si impurities, which have a valence difference of 3 with respect to Fe.[25] The valence difference is 2 for Al. Terakura[32] has discussed the *d*-band filling and emptying effects for nontransition element impurities in Fe and concludes that these nearly cancel each other. Simple dilution of the *d*-electron contribution to the hyperfine field on the muon, if that were the main contribution, would lead to $\Delta B_{\rm hf}/cB_{\rm hf}$ of -1.0 which is three times larger than the data indicate. The apparent disagreement can be resolved with an explanation in terms of the contribution from conduction electrons.

NMR and Mössbauer measurements have found that the hyperfine field on Fe nuclei at sites nearest neighbor to Al impurities is less negative by 7% and this has been attributed to a small reduction in the local, negative conduction-electron polarization.[29] At the Al site, the conduction-electron polarization is negative due to the negative hyperfine field on the Al.[40] From a different point of view, Stearns has treated the pickup of conduction-electron polarization at impurities from the neighboring Fe atoms in terms of the volume misfit of the impurity atom.[44,45] This effect is small for the Al impurity and can be neglected. Referring to the theoretical results calculated by Terakura,[32] the fractional change in the *s*-electron polarization within the Wigner-Seitz sphere at the Al is $+0.08$ and the *p*-polarization change is -0.03, for a total of $+0.05$. These findings can be used to make a prediction for the change in the average $B_{\rm hf}$ for muons per unit concentration of Al impurity, taking into account the free-electron spin-density enhancement factor of 9.8

$$\Delta B_{\rm hf}/c = 9.8\frac{8\pi}{3}(0.05\times 2\mu_{\rm B}/a_0^3) = 3.3 \text{ kG} \quad . \quad (11)$$

This is equivalent to $\Delta B_{\rm hf}/cB_{\rm hf} = -0.30$ and is close to the measured asymptotic value of -0.35 ± 0.03.

The average change in the hyperfine field at the Fe sites in Fe(Al) has been given by several authors.[46,47] The fractional change is in the range -0.4 to -0.5.

Nishida *et al.*[35] have recently measured $B_{\rm hf}$ for Fe doped with 5-at.% Si at 300 K. They find $\Delta B_{\rm hf}/cB_{\rm hf} = -0.24$. This is the same as the value we find for our 301 K measurements on Fe(Al). Although the asymptotic limit was not checked in the Fe(Si) measurements, this result suggests an insensitivity to the valence difference between Al and Si.[30] The magnetic properties of Fe(Al) and Fe(Si) are also similar.[27]

Our explanation for the change in the hyperfine field on muons assumes that distortions in the localized *d*-wave-function amplitudes at interstitial sites near the Al impurity can be neglected. This is based on the assumption that local changes in electron-spin density associated with these states are not enhanced when the muon is present, as is the case for itinerant states. Thus we are assuming that the μ^+ impurity acts in a manner similar to Al and Si impurities by creating minimal magnetic disturbance in its vicinity. Nevertheless, we cannot completely rule out the possibility that the weak dependence of $B_{\rm hf}$ on Al concentration may arise in part from a large increase in the minority-spin *d*-like wave functions at interstitial sites near the Al. It would be interesting, therefore, to investigate the systematic behavior of $B_{\rm hf}$ for other nonmagnetic impurities in Fe as well.

Owing to the apparently extreme sensitivity of $B_{\rm hf}$ to attractive defect potentials, it would be interesting to investigate the systematic effects of dislocations and impurities such as C, O, and N in Fe alloy samples. Our interpretation predicts a logarithmic dependence of the temperature of inflection in Fig. 2 on the defect concentration. This could be tested with deformed alloys.

Our basic conclusion is that one obtains consistency by treating both the local magnetic perturbation around Al impurities[29] and the hyperfine field on the muon[3] as problems of conduction-electron screening and spin-density perturbation. It is hoped that these measurements will motivate more fundamental calculations for determining the origins of the muon hyperfine field and the local muon potential, such as finite cluster calculations treating the ternary system μ^+-Al in Fe.

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*Present address: Nucl. Res. Cen. Univ. of Alberta, Edmonton, Alberta, Canada T6G 2N5.
†Present address: Siemens Corp., Cherry Hill, N. J. 08003.

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