FROM THE CURRENT LITERATURE

Muon spin relaxation in crystals with defects

A. I. Morozov and A. S. Sigov

Institute of Radio Engineering, Electronics, and Automation
(Submitted 29 April 1993)
Usp. Fiz. Nauk **163**, 75–88 (September 1993)

A study is made of the behavior of a positive muon in the matrix of a real, nonmagnetic metal containing defects. The temperature dependence is found for the relaxation rate of the muon spin due to the dipole-dipole interaction between the magnetic moment of the muon and the magnetic moment of the nuclei of the matrix. Data from μSR experiments with a series of metals are analyzed and it is shown that the data can be consistently interpreted within the framework of a unified approach that explains the observed muon spin relaxation by the capture of the muon in a trap.

1. INTRODUCTION

The same abbreviation μSR is used to designate muon spin resonance, muon spin rotation, and muon spin relaxation. The method of μSR is effective for the study of local magnetic fields and their time dependence in crystals. This method makes it possible to determine a number of important characteristics of magnets and superconductors. A large numbers of papers have been devoted to a description of the technique of μSR experiments (see, e.g., the reviews, Refs. 1 and 2.). A polarized beam of positive muons produced by the decay of π mesons is incident on the sample. When they enter the sample the muons are thermalized in a time of the order of 10^{-12} to 10^{-13} s.

The muons are then depolarized under the action of random magnetic fields. The time dependence of the muon polarization $P(t)$ is determined by observations of the asymmetry of the emission of the positrons produced by the decay of the muon into a positron, an electron neutrino and a muon antineutrino

$$\mu^+ \to e^+ + \nu_e + \bar{\nu}_\mu$$

with a characteristic time $\tau_\mu = 2.2\ \mu$s.

In the case of measurements in a transverse magnetic field (perpendicular to the initial polarization of the beam) the time dependence $P(t)$ is used to determine the precession frequency and the muon spin relaxation rate, while in measurements in a longitudinal field, and in particular, in zero field, only the latter is determined.

However, to obtain information on the local magnetic fields it is necessary to know the behavior of a muon in a crystal: whether it is captured in a trap or if it moves through the crystal. Qualitatively, a positive muon can be regarded as a very light hydrogen isotope that retains its mobility in an ideal crystal even at the lowest temperatures, tunneling quantum mechanically from one equivalent interstitial site to another.

In the case of the fast motion of a muon through a crystal the random field acting on its spin is effectively averaged and the relaxation rate decreases. This is the well-known effect of motional narrowing of resonance lines.

In nonmagnetic metals the muon spin is acted on by the magnetic field that is produced by the dipole moments of the matrix nuclei, which remains practically unchanged during the time of observation. The fields that act on the muon in neighboring interstitial sites are essentially uncorrelated. In this case the relaxation rate will be the greatest when the muon remains in the same interstitial site during its entire lifetime after thermalization until it decays.

Experimental data have recently been obtained for the frequency of hopping of hydrogen between neighboring equivalent interstitial sites in a metal matrix. Since the muon is nine times lighter than the proton, its hopping frequency should be much greater. Even if we use the minimum estimate obtained for hydrogen for this quantity, it turns out that during the time of observation, a time of the order of 10 μs, there can be no significant relaxation of the muon spin.

From this result it follows that in a real crystal the muon spin relaxes because of the nonideality of the crystal, i.e., the crystal contains traps. As will be shown below, any defect of the crystal lattice can act as a trap. When the temperature is lowered below some characteristic value the muon in the equilibrium state will with overwhelming probability be captured in a trap.

However, the initial spatial distribution of the muons is not an equilibrium distribution. According to the "standard model", the muon after thermalization can occupy with equal probability any of the equivalent interstitial sites. Therefore, the relation between the time of capture of the muon by a trap and its spin relaxation time in that trap plays an important role.

An analysis of μSR experimental data in pure metals shows that almost all the data can be accounted for if it is assumed that the cause of muon spin relaxation is the capture of the muon by point defects. Then a matter of importance is the possibility of a point defect creating several energy minima (traps) of different depths for the muon. Frequently, a muon must overcome a potential barrier to be captured in a trap. In this case, the fraction of the muons that are captured in such a trap will be appreciable only at temperatures where the probability of surmounting the potential barrier is sufficiently high.

The technique of μSR can be used under certain conditions to study the quantum mechanical diffusion of a muon. In the case of metals this possibility is practically unique (the other objects of study are the metal hydrides), since the ninefold smaller mass than that of hydrogen increases by a large factor the quantum mechanical contribution to the diffusion coefficient of the muons. We shall discuss how the data on the diffusion coefficient can be extracted from the results of μSR experiments.

In Sec. 2 we consider the behavior of a muon in a pure crystal. In Section 3 we describe the interaction between a muon and point defects and the bound states that are formed. Section 4 gives a description of muon spin relaxation in a crystal with traps, and in Sec. 5 we make a comparison with experimental data. Finally, we present a synopsis of the work and our conclusions.

2. MUON SPIN RELAXATION IN A PURE CRYSTAL

2.1. Diffusion mechanism

Let us first consider the nature of the motion of a muon in a hypothetical defect-free crystal. At the lowest temperatures the muon will tunnel quantum mechanically from one equivalent interstitial site to another, and it can be described in the language of a Bloch wave. The characteristic band width of hydrogen in niobium, determined on the basis of experiments on the absorption of ultrasound and inelastic scattering of neutrons, is 1–10 K (Refs. 3,4). Because the muon mass is nine times smaller than that of hydrogen the width of the muon band, $\zeta=2z\varepsilon_0$, where z is the number of nearest-neighbor equivalent interstitial sites and ε_0 is the tunneling matrix element for the muon, must be considerably larger and reach values of tens of degrees. In a pure metal the mean free path of a muon in the region of band motion is determined by its scattering by conduction electrons. These processes have been examined in Refs. 5–7. In the temperature range $T\gg\zeta$ the mean free time τ of a muon is

$$\tau^{-1}=2\pi gT/\hbar, \tag{1}$$

where $g\approx 2N^2(0)V_0^2$, $N(0)$ is the density of electrons at the Fermi surface, and V_0 is the amplitude for scattering of an electron by a muon. For characteristic metallic values of $N(0)$ and V_0, we find $g\sim 0.1$–1.

Let us estimate the muon diffusion coefficient D using the kinetic relation

$$D=\langle v^2\rangle\tau_{tr}/3, \tag{2}$$

where $\langle v^2\rangle$ is the mean square velocity of the muon and τ_{tr} is the transport time of free flight of the muon. For $T>\zeta$ we find $\tau_{tr}\sim\tau$ and $\langle v^2\rangle=\zeta^2d^2/\hbar^2$, where d is the interatomic spacing. Then[6,7]

$$D=\zeta^2d^2/gT\hbar. \tag{3}$$

The interaction of electrons with a muon also leads to a renormalization of the muon band width in a metal—the electron polaron effect.[8] The renormalized value of ζ is

$$\zeta=\zeta_0[\max(T,\zeta_0)/E_0]^\beta, \tag{4}$$

where ζ_0 is the muon band width in the absence of the interaction with the electrons, E_0 is the width of the conduction band, and $\beta\sim g$. Therefore, for $T>\zeta$ the temperature dependence of the diffusion coefficient has the form[8]

$$D\propto T^{2\beta-1},\quad \beta\ll 1.$$

In the temperature range $T\gg\zeta$, we have, according to Refs. 6 and 7

$$\tau^{-1}=2\pi gT^2/\hbar\zeta, \tag{5}$$

$$\tau_{tr}\sim\tau,\quad a\langle v^2\rangle=T\zeta d^2/\hbar^2;$$

and consequently

$$D=\zeta^2d^2/gT\hbar T^{-1}, \tag{6}$$

since ζ no longer depends on T when $T<\zeta$.

In the case of a semimetal, the dependence $D(T)$ is more complicated.[7] In the superconducting phase, because of the formation of a gap Δ in the spectrum of electron excitations, the mean free time τ_{sc} due to muon scattering by electrons is

$$\tau_{SC}=\tau[1+\exp(\Delta/T)]/2, \tag{7}$$

and the quantity $\max(T,\zeta_0)$ in formula (4) is replaced by $\max(T,\zeta_0,\Delta)$ (Ref. 9).

Thus, for $T\ll\Delta$ the scattering of a muon by electrons in a superconductor is unimportant, since the number of electronic excitations is exponentially small, and, as in an insulator, the main role is played by scattering by phonons. Since for $T\ll\Theta$, where Θ is the Debye temperature, the mean free path of quantum particles due to scattering by phonons is much greater than the interatomic spacing d (Refs. 10, 11), in a pure superconductor at temperatures $T\ll\Delta$ band motion of the muons occurs. The diffusion coefficient of the muons depends on the temperature as[10,11]

$$D\propto T^{-9}. \tag{8}$$

Let us turn now to a consideration of the motion of a muon in a normal metal. As the temperature increases with $T > T_0'$ the quantity τ^{-1} exceeds ζ and mean free path of the muons becomes smaller than the interatomic spacing. Here the description in the language of Bloch functions is inapplicable.

With a further increase in temperature, $T > T_h > T_0'$, the diffusion of a muon can be regarded as a Markovian process of quantum mechanical hopping between neighboring interstitial sites.[12] At higher temperatures the main diffusion mechanism is the classical barrier-surmounting mechanism. A consistent description of the diffusion coefficient does not exist for the region $T_0' < T < T_h$.

An analysis of the diffusion coefficient of light particles in a metal that takes into account interactions with electrons and with phonons has been carried out in Ref. 8.

In the temperature range $T\ll\Theta$ the role of the interaction with phonons reduces to a polaron narrowing of the muon band:

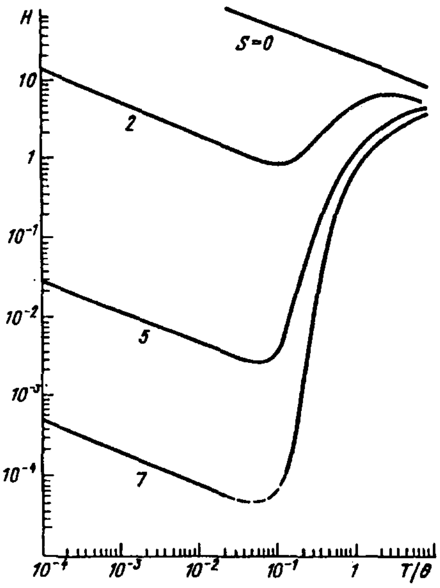

FIG. 1. Temperature dependence of the normalized hopping frequency for $\beta=0.3$ and $E_0/\theta=100$.

$$\zeta_0=\zeta_{00}\exp(-S), \tag{9}$$

where ζ_{00} is the band width in the absence of the phonon interaction and S is the dimensionless muon-phonon coupling constant:

$$S=u_p^2/w_0^2, \tag{10}$$

where u_p is the displacement of a lattice atom from a site nearest the muon and w_0 is the amplitude of the zero-point oscillations of the atom.

In the temperature range $0.1\Theta<T<\Theta$ there is a sharp increase in the diffusion coefficient due to the fast increase in the rate of quantum mechanical hopping between adjacent interstitial sites. For $T>\Theta$ the quantum diffusion becomes activated, as in the case of insulators.

A compact analytical expression for the hopping probability with allowance for interactions with the electrons and phonons is lacking, but the results of a numerical calculation carried out by Kondo[8] are shown in Fig. 1.

We can estimate the maximum time $\tau_h^{\max}$ between two hops as

$$\tau_h^{\max}=\hbar T_{\min}/z\varepsilon_0^2, \tag{11}$$

where $T_{\min}$ is the temperature corresponding to the minimum probability of a hop (Fig. 1). Its value is $T_{\min}=0.1\Theta$.

2.2. Relaxation rate

Let us now consider the muon spin relaxation rate in each of the above-mentioned temperature intervals. In a nonmagnetic metal the relaxation is due to the dipole-dipole interaction between the magnetic moment of the muon and the magnetic moments of the nuclei of the matrix, while the characteristic relaxation time in the region of band motion is given by the time of scattering of a Bloch wave with a spin flip due to this interaction.[13] The analogous problem for a conduction electron in a semiconductor has been examined in Ref. 14.

In the case of uncorrelated nuclear spins the muon spin relaxation time τ_s is given by the formula

$$\tau_s^{-1}(\mathbf{k})=\frac{2\pi}{\hbar\Omega}\int|V_{1/2,-1/2}(\mathbf{k}-\mathbf{k}')|^2\times\delta(\varepsilon(\mathbf{k})-\varepsilon(\mathbf{k}'))\frac{d\mathbf{k}'}{(2\pi)^3}, \tag{12}$$

where $\mathbf{k}$ and $\mathbf{k}'$ are the initial and final quasimomenta of the muon, Ω is the volume of the unit cell, $\varepsilon(\mathbf{k})$ is the muon dispersion relation, and $V_{1/2,-1/2}(\mathbf{k}-\mathbf{k}')$ is the amplitude for scattering of a muon by an individual nucleus with a spin flip.

If $T>\zeta$, then the characteristic values of $\mathbf{k}$ are of the order of the Brillouin momentum k_B and in order of magnitude τ_s are equal to

$$\tau_s^{-1}=\sigma_0\hbar/\zeta, \tag{13}$$

where σ_0^{-1} is the muon relaxation time in the absence of diffusion, and σ_0 $\langle\delta H\rangle$, where $\langle\delta H\rangle$ is the characteristic magnitude of the fluctuations of the magnetic field.

The dependence $\tau_s(T)$ in this temperature range is due to the temperature dependence of ζ (see formula (4)). Thus

$$\tau_s^{-1}=\frac{\sigma_0^2\hbar}{\zeta_0}\left(\frac{T}{E_0}\right)^{-\beta}. \tag{14}$$

For $T\ll\zeta$ the characteristic thermal momentum of the muon is $k\sim k_B(T/\zeta)^{1/2}$. In this case from Eq. (12) we obtain[13]

$$\tau_s^{-1}=\sigma_0^2\hbar T^{1/2}/\zeta^{3/2}. \tag{15}$$

This same temperature dependence for $\tau_s(T)$ was predicted in the work of Kondo[15] on the basis of an assumption of the form of the correlation function of the dipole field.

For characteristic values $\sigma_0\sim10^5$–$10^6\,\mathrm{s}^{-1}$, $\zeta\sim1$ meV, $\beta\sim0,1$, $T\sim1-10$ K and $E_0\sim10^4-10^5$ we obtain the estimate $\tau_s\gtrsim10$ K, which is many orders of magnitude greater than the time of observation $t_0\sim10$ μs. Consequently the muon spin relaxation in a pure metal in the low-temperature region must be experimentally unobservable.

In the range of temperatures where the diffusion of muons is a succession of uncorrelated hops from one interstitial site to another, the time dependence of the muon polarization for an experiment in a transverse magnetic field is described by the formula[16]

$$P(t)\equiv P(0)G(t)=P(0)\exp\{-2\sigma_0^2\tau_h^2\times[\exp(-t/\tau_h)-1+(t/\tau_h)]\}. \tag{16}$$

When $\tau_h\sigma_0\gg1$ then $G(t)$ takes on a Gaussian shape

$$G(t)=\exp(-\sigma_0^2t^2), \tag{16a}$$

and for $\tau_h\sigma_0 \ll 1$ it is a Lorentzian

$$G(t)=\exp(-2\sigma_0^2\tau_h t). \tag{16b}$$

Here it is assumed that the dipole fields acting on the muon spin in neighboring interstitial sites are not correlated.

For the case of relaxation in a zero magnetic field there is no simple analytical expression for the function $G(t)$ for an arbitrary relation between σ_0 and τ_h. In the limiting case $\sigma_0\tau_h \gg 1$, $G(t)$ is described by the formula of Kubo and Toyabe[17]

$$G(t)=\tfrac{1}{3}+\tfrac{2}{3}(1-2\sigma_0^2t^2)\times\exp(-\sigma_0^2t^2). \tag{17}$$

For measurements in both longitudinal and transverse magnetic fields the muon spin relaxation rate t_s^{-1} in the region of hopping diffusion can be written as

$$\tau_s^{-1}=2\sigma_0^2\tau_h(2\sigma_0\tau_h+1)^{-1}. \tag{18}$$

Let us estimate the value of t_s^{-1} for the maximum value t_h^{max} given by formula (11):

$$\tau_s^{-1}=2\sigma_0^2\hbar T_{min}/\zeta\varepsilon_0. \tag{19}$$

For the values given above for σ_0 and ζ and for $T_{min}\sim 20$–50 K we obtain $\tau_s\sim 0.1$–10 s, which is much greater than the observation time.

Thus the observation of the muon spin relaxation rate in a pure metal is possible only when the value of ε_0 for the muon in the metal has the anomalously low value of $\varepsilon_0 \lesssim 10^{-3}$ K.

For the real values $\varepsilon_0\sim 1$ to 10 K it is not possible to observe the muon spin relaxation rate in an ideal crystal.

3. INTERACTION OF A MUON WITH POINT DEFECTS

On the basis of the discussion of the last Section it can be concluded that the muon spin relaxation rate observed experimentally is due to the presence in the crystal of traps, which can be any point defect in the metal.[18,19]

Of course, a muon can also be captured by dislocations and planar defects of the crystal lattice. However, then the muon can move rapidly along the dislocation or in the plane of the two-dimensional stacking fault. Therefore the effect of averaging of the random field at the muon spin is not eliminated.

The long-range part of the interaction potential between the muon and a point defect (as between any two point defects) is made up of an elastic interaction, i.e., an indirect interaction via acoustic phonons and an interaction via Friedel oscillations in the electron density, caused by the defects, i.e., an indirect interaction via the conduction electrons:

$$W(\mathbf{R})=W_{elas}(\mathbf{R})+W_{el}(\mathbf{R}). \tag{20}$$

Both of these long-range components fall off with the distance R between the muon and the defect as R^{-3}.

The elastic interaction at a distance $R\gg d$ has the form

$$W_{elas}(\mathbf{R})=W(\mathbf{n})\Omega/R^3, \tag{21}$$

where $\mathbf{n}=\mathbf{R}/R$ and $W(\mathbf{n})$ changes sign with a change in the direction of the vector $\mathbf{n}$ relative to the crystallographic axes.

The interaction via the Friedel oscillations of the electron density can be written in the Born approximation as

$$W_{el}(\mathbf{R})=N(0)\Omega V_0(2k_F)V_1(2k_F)\cos(2k_FR)\times(2\pi\tilde{\varepsilon}^2(2k_F)R^3)^{-1}, \tag{22}$$

where k_F is the Fermi momentum of the electrons, $V_1(\mathbf{k})$ is the amplitude for scattering of an electron by a point defect, and $\tilde{\varepsilon}(k)$ is the permittivity of the metal.

For $R\sim d$, both interactions have energies of the order of $\tilde{W}=0.01$–0.1 eV for values of the physical parameters characteristic of metals. Because $\cos(2k_FR)$ and $W(\mathbf{n})$ change sign regardless of the sign of the short-range part of the interaction between the muon and the point defect, there is a set of interstitial sites with $W(\mathbf{R})<0$, where the state with the highest binding energy W_0 is located at a distance $R\sim d$ from the defect. Thus any point defect in a metal creates a large number of bound states for a muon.

The difference in energy between muons in localized interstitial sites i and j is given by

$$\zeta_{ij}=\sum_m (W(\mathbf{r}_i-\mathbf{r}_m)-W(\mathbf{r}_j-\mathbf{r}_m)), \tag{23}$$

where the summation is over all the point defects, $\mathbf{r}_m$ are their coordinates, and $\mathbf{r}_{ij}$ are the coordinates of the interstitial site. The mean square spread in the energies of neighboring interstitial sites, due to the presence of randomly distributed impurities with a concentration x, is of the order of

$$(\langle\zeta^2\rangle)^{1/2}=x\tilde{W}$$

and for $x\approx 10^{-4}$–10^{-5} can be much less than ζ and does not inhibit band motion of the muon far from the defect.

Let us now consider the equilibrium spatial distribution of the muons in a crystal with defects. Obviously, at a high temperature the muons are distributed with equal probability over the interstitial sites of a given kind, while at low temperatures they are in the bound state with the lowest energy.

Let us estimate the temperature T_0 of capture of muons by defects starting from the following simple model.[18] The average value of $W(\mathbf{n})$ over a unit sphere is equal to zero, and $\cos(2k_FR)$ oscillates rapidly with a characteristic period of the order of d. Therefore we assume that in a spherical shell of radius R and a thickness dR constructed around the defect there will be $4\pi R^2 dR/\Omega$ states, whose energies are equally distributed in the interval from $-\tilde{W}\Omega/R^3$ to $+\tilde{W}\Omega/R^3$. The minimum distance between the muon and the defect is $r_{min}\sim d$, and the maximum distance is $r_{max}\sim x^{-1/2}d$. The probability of a particle being found in a particular spherical shell is

$$dw(R)=\int_{-\infty}^{\infty} dEA\exp\left(-\frac{E}{t}\right)\times\theta\left(\frac{\tilde{W}\Omega}{R^3}-\left|E\right|\right)$$

$$\times\frac{2\pi R^5 dR}{\Omega^2\widetilde{W}}$$

$$=\frac{4\pi TAR^5 dR}{\Omega^2\widetilde{W}}\,\mathrm{sh}\,\frac{\widetilde{W}\Omega}{TR^3}, \qquad (24)$$

where A is found from the normalization condition. This model takes into account the presence of a large number of bound states for the muon, but does not include many-particle effects in the analysis. For $T\gg T_0$ the average distance between the muon and a defect is $\langle r\rangle \sim r_{\max}$, and for $T\ll T_0$ it is $\langle r\rangle\sim r_{\min}$. The transition from one limiting case to the other occurs in the interval of temperatures $T_0/|\ln x|$ near the temperature

$$T_0=W_0/|\ln x|. \qquad (25)$$

The principal role in the case of potential (20) is played by the states with the lowest energies, and the fact that there are a large number of bound states plays little role in the determination of T_0. The fraction of muons in states with energies $W(\mathbf{R})<-T$ is equal to

$$\varkappa=1-\left[1+\gamma x\left(\frac{T}{W_0}\right)^2\exp\left(\frac{W_0}{T}\right)\right]^{-1}, \qquad (26)$$

where $\gamma\sim 1$. For $T\gg T_0$, the value of $\varkappa$ is practically zero, while for $T\ll T_0$ it is equal to unity with exponential accuracy.

4. MUON SPIN RELAXATION RATE IN A CRYSTAL WITH TRAPS

4.1. Muon diffusion

Let us consider first the motion of muons in a crystal with defects. As noted above, there exists a region of the crystal in which the characteristic values of

$$W_i=\sum_m W(\mathbf{r}_i-\mathbf{r}_m) \quad \text{and } \zeta_{ij}$$

do not exceed ζ. In this region of space for $T\gtrsim\zeta$ the behavior of the muon does not differ qualitatively from that in the pure crystal. It is only necessary to take into account an additional mechanism of scattering of the muon by nonuniformities of the crystal lattice. For low defect concentrations this region occupies the entire volume of the crystal except for a sphere of radius

$$\tilde{r}=d(\widetilde{W}/\zeta)^{1/3}, \qquad (27)$$

about each defect. Since $\cos(2k_F R)$ oscillates rapidly over atomic distances, the value of ζ_{ij} is comparable to ζ practically up to the boundary.

Near the defect, where $|W_i|$, $|\zeta_{ij}|>\zeta$, the motion of the muon takes on the nature of transitions between states that with good accuracy are localized in the corresponding interstitial sites. The nonequivalence of the interstitial sites makes possible one-phonon transitions between them. In order of magnitude the probability of a transition from an interstitial site i into a neighboring crystallographically inequivalent interstitial site j of a given type is[20]

$$(\tau_{ij,\mathrm{h}}^{-1})_{\mathrm{ph}}=\varepsilon_0^2\zeta_{ij}\widetilde{E}\times\{\hbar\theta^3[1-\exp(-\zeta_{ij}/T)]\}^{-1}, \qquad (28)$$

where $\widetilde{E}$ is an energy on the atomic scale and

$$\varepsilon_0=\varepsilon_{00}[\max(T,\varepsilon_{00},\zeta_{ij})/E_0]^{\beta}, \qquad (29)$$

where ε_{00} is the bare value of the tunneling matrix element.

For $T\gg|\zeta_{ij}|$ we find $(\tau_{ij,\mathrm{h}}^{-1})_{\mathrm{ph}}\propto T^{1+2\beta}$. Neglecting the quantity $\beta\ll 1$, we obtain the relation $(\tau_{ij,\mathrm{h}}^{-1})_{\mathrm{ph}}\propto T$, which nearly always has been interpreted experimentally as the observation of one-phonon processes. However, this same temperature dependence of $\tau_{ij,\mathrm{h}}$ is also obtained for transitions between interstitial sites caused by the interaction between the muon and electrons. In this case[21,22]

$$(\tau_{ij,\mathrm{h}}^{-1})_{\mathrm{el}}=4\pi\beta\varepsilon_0^2\times\{\hbar\zeta_{ij}[1-\exp(-\zeta_{ij}/T)]\}^{-1}. \qquad (30)$$

For $T\gg|\zeta_{ij}|$ the value of $(\tau_{ij,\mathrm{h}}^{-1})_{\mathrm{el}}$ is also proportional to the temperature, and the ratio of the transition rates is of the order of

$$(\tau_{ij,\mathrm{h}}^{-1})_{\mathrm{ph}}/(\tau_{ij,\mathrm{h}}^{-1})_{\mathrm{el}}\sim\zeta_{ij}\widetilde{E}/4\pi\beta\Theta^3. \qquad (31)$$

In the region of temperatures $T\ll\Theta$ the principal mechanism that induces transitions of the muon between interstitial sites in a normal metal is the interaction with conduction electrons, and therefore the observation that $\tau_{\mathrm{h}}^{-1}\propto T$ is not evidence for the one-phonon mechanism.

In a superconductor with $T\ll\Delta$, where the number of electronic excitations is exponentially small, the phonon transition mechanism may become the determining one.

4.2. Muon spin relaxation

Let us now examine muon spin relaxation in a crystal with defects. Because the interstitial sites are no longer equivalent and the motion of the muons near a defect is different from that far the defect we cannot describe the behavior of the muon polarization by a function of the type (16) with a single characteristic time τ_{h}. Unfortunately, in the work of Refs. 23 and 24 only the function $\tau_{\mathrm{h}}(T)$ was calculated in this model, and not $\lambda(T)$, the experimentally measurable muon spin relaxation rate as a function of the temperature.

4.2.1. Two-state model

This model is based on the assumption that the muon can be found either in the free state or in the trapped state. Each state is characterized by its own relaxation rate: σ_f and σ_{tr}, respectively. The characteristic time of capture of a muon by a trap is τ_1, while the characteristic time of release of a muon from a trap is τ_2, and the concentration of traps is x.[25]

It is clear that within this model the large number of bound states that are created by one defect is replaced by one effective trap.

Let us consider the relaxation function $G(t)$ in the framework of the given model:

$$G(t)=\sum_{n=1}^{\infty}(G_{n,f}(t)+G_{n,\mathrm{tr}}(t)), \qquad (32)$$

where the functions $G_{n,f}(t)$ and $G_{n,\mathrm{tr}}(t)$ obey the following recursion relations:

$$G_{1,f}(t)=(1-\varkappa(0))\exp(-t/\tau_1)G_{0,f}(t); \quad (33)$$

$$G_{1,tr}(t)=\varkappa(0)\exp(-t/\tau_2)G_{0,tr}(t); \quad (34)$$

$$G_{n+1,f}(t)=\frac{1}{\tau_2}\int_0^t G_{n,tr}(u)\exp[-(t-u)/\tau_1] \times G_{0,f}(t-u)\mathrm{d}u; \quad (35)$$

$$G_{n+1,tr}(t)=\frac{1}{\tau_1}\int_0^t G_{n,f}(u)\exp[-(t-u)/\tau_2] \times G_{0,tr}(t-u)\mathrm{d}u, \quad (36)$$

and describe the relaxation of the spins of a group of muons that are found n times in the free and the trapped states, respectively. In the case of relaxation in a transverse magnetic field the function $G_{0,f(tr)}(t)$ is given by formula (16a), and for relaxation in zero magnetic field it is given by formula (17).[26]

The quantity $\varkappa(0)$ is the fraction of trapped muons at the initial instant of time (immediately after thermalization). According to the standard model, the value of $\varkappa(0)$ is proportional to the number of interstitial sites that are traps, i.e., $\varkappa(0)=x$, and for $x\ll 1$ is negligibly small.

For the case where, because of the same reasons cited in Section 2 the relaxation of the spins of the free muon can be neglected, the system of equations is obtained from Eqs. (32)–(36) with $G_{0,f}(t)\equiv 1$. The solution of the system of equations (32)–(36) is found by the method of Laplace transforms.[25] The optimum values of the parameters σ_f, σ_{tr}, τ_1, and τ_2 are found by a comparison of the experimentally determined $G(t)$ with the calculated function.

However, as shown in Refs. 13 and 27, there exists a temperature range in which the expression for the muon spin relaxation rate λ can be obtained analytically.

Within the standard model the initial spatial distribution of muons is a nonequilibrium distribution, since in equilibrium the muon has a high probability of occupying an interstitial site that corresponds to a trap. If the time τ_1 is much less than the muon spin relaxation time τ_s, then the spatial distribution relaxes to the equilibrium distribution much faster than the muon spin, and experimentally it can be regarded as an equilibrium distribution. Then because of ergodicity the fraction of captured muons $\varkappa$ is

$$\varkappa=\tau_2/(\tau_1+\tau_2)=1-[1+x\exp(W_0/T)]^{-1}, \quad (37)$$

where W_0 is the binding energy of a muon in a trap and the muon spin relaxation rate in the two-state model is given by the expression

$$\tau_s^{-1}=\varkappa\tau_{s,tr}^{-1}+(1-\varkappa)\tau_{s,f}^{-1}. \quad (38)$$

The relaxation rate $\tau_{s,f}^{-1}$ in the free state is negligible, while the rate in the trapped state is given by formula (18), where

$$\sigma_0\equiv\sigma_{tr} \quad \text{and} \quad \tau_h\equiv\tau_2.$$

If it is assumed that τ_2 has the usual exponential dependence on T of the form

$$\tau_2=\tau_0\exp(W_0/T), \quad (39)$$

where τ_0 is a constant, then we can introduce the characteristic temperature T_1, for which $\tau_2(T_1)\sigma_{tr}=1$:

$$T_1=W_0/|\ln(\sigma_{tr}\tau_0)|. \quad (40)$$

If $T_1<T_0$, i.e.,

$$x\gg\sigma_{tr}\tau_0, \quad (41)$$

then the condition of ergodicity is satisfied over the entire temperature range, and the τ_s^{-1} increases sharply with decreasing temperature, for $T=T_1$ with $\varkappa=1$, and

$$\tau_s^{-1}=\tau_{s,tr}^{-1}=2\sigma_{tr}^2\tau_2(2\sigma_{tr}\tau_2+1)^{-1}. \quad (42)$$

The function $\tau_s^{-1}(T)$ has the form shown in Fig. 2, and it remains practically unchanged as the concentration increases up to the point where inequality (41) is violated.

In the opposite case, $T_1>T_0(x\ll\sigma_{tr}\tau_0)$, ergodicity can be used in the region of high temperatures $T>T^*(\tau_s(T^*)=\tau_1)$, and in the entire range of interest to us $t\lesssim T_1$, the spatial distribution function of the muons is quite far from equilibrium. To obtain information on the muon spin relaxation rate in this temperature range we carried out a numerical simulation and found the solution to the system of equations (32)–(36) for a wide range of values of τ_1 and τ_2 (in units of σ_{tr}^{-1}). The relaxation rate λ was determined by approximating the function $G(t)$ by the functions $\exp(-\lambda^2t^2)$ and $\exp(-\lambda t)$ (Ref. 26).

Over the entire investigated regirangeon of values of τ_1 and τ_2 we find that with an accuracy of the order of 10% λ is well approximated by the formula

$$\lambda=[\tau_1+\tau_s]^{-1}$$
$$=\{\tau_1\{+[(\tau_1+\tau_2)(1+2\sigma_{tr}\tau_2)/2(\tau_2\sigma_{tr})^2]\}^{-1}. \quad (43)$$

Since in the simulation we did not use a specific form for the functions $\tau_1(T)$ and $\tau_2(T)$, formula (43) is applicable for an arbitrary temperature dependence of τ_1 and τ_2.

For $T<T_1$, where $\sigma_{tr}\tau_2\gg 1$,

$$\lambda=\{\tau_1+[(\tau_1+\tau_2)/\tau_2\sigma_{tr}]\}^{-1}, \quad (44)$$

and λ will be observed to increase with decreasing temperature for $T=T_0$. For $T<T_0$, we have $\tau_2\gg\tau_1$, σ_{tr}^{-1} and the release of the muon from the trap can be neglected. Then

$$\lambda=(\tau_1+\sigma_{tr}^{-1})^{-1}. \quad (45)$$

When τ_1 and τ_2 are both constant, then the function $\lambda(T)$ is as shown in Fig. 2. Since τ_1^{-1} x the value of λ that corresponds to the low-temperature plateau increases with trap concentration, and assumes a constant value equal to σ_{tr} for $\tau_1\ll\sigma_{tr}^{-1}$. However, if τ_1 depends on the temperature, then one can recover the function $\tau_1(T)$ from the temperature dependence of λ below T_0 and draw conclusions about the temperature dependence of the diffusion coefficient of muons in a metal.

In addition it should be noted that in a real metal, as will be shown below, the time τ_1 is not the characteristic time for a muon to encounter a trap, since not each encounter results in capture of the muon by the trap. There-

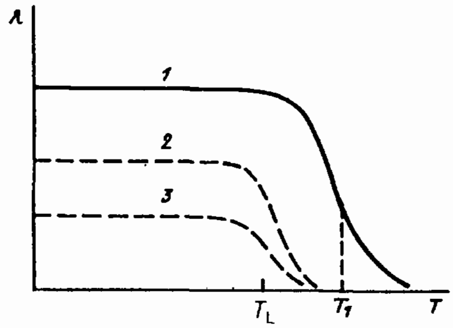

FIG. 2. Theoretical temperature dependence of the muon spin relaxation rate for $T_1 < T_0(1)$ and $T_0 < T_1(2,3)$; $x^{(2)} > x^{(3)}$.

fore μSR data cannot, unfortunately, give information on the value of the diffusion coefficient in a pure metal.

4.2.2. Beyond the two-state model

Let us see what sort of qualitative factors were not taken into account in the model investigated above. As noted above, each defect creates about itself a large number of bound states. A trap is understood to be an interstitial site with an energy $W_i < -T$. We note that in the higher temperature region the main contribution to the muon relaxation comes from the deepest minimum closest to the defect, but at low temperatures the muon is trapped in an interstitial site that is rather distant from the defect. Here the quadrupole interaction with the defect becomes much weaker. This is the reason for the difficulty in identifying the type of interstitial site in which the muon is localized. While the type of interstitial site can be determined uniquely at higher temperatures, at low temperatures such a conclusion cannot be made,[28] or else the experimental data are interpreted as a change in the type of interstitial site.[29–31]

Since the energy of interaction of a muon with a defect falls off quite rapidly with distance from the defect, the deepest energy minimum is separated from the next one in depth, but the shallower minimum (or minima) will be separated by a rather high potential barrier (Fig. 3). In this case the deepest minimum may be a trap only at low temperatures if it in general lies in the region of the static distortion of the energy levels, $|\mathbf{r}_i - \mathbf{r}_m| < \tilde{r}$.

The potential barrier is penetrable by a muon only at rather high temperatures, while at low temperatures the muon is reflected from it with overwhelming probability. Therefore the capture of a muon in a deep energy minimum and the relaxation of the muon spin is observed at high temperatures. As the temperature is raised further, the relaxation rate λ falls off because of the decrease in the time τ_2 for the release of a muon from a trap. The characteristic form of $\lambda(T)$ in this case is shown in Fig. 4. The low-temperature plateau on the curve of $\lambda(T)$ is due to the contribution from shallower energy minima and may be absent if the muon is incident in the region of a small static distortion of the levels. This dependence of $\lambda(T)$ has been observed in Al and Au with Gd and Er impurities.[32–34]

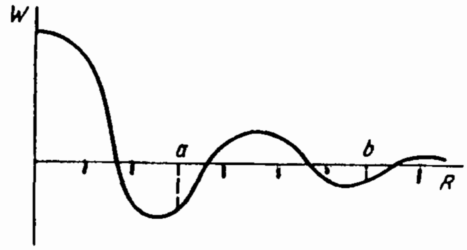

FIG. 3. Potential acting on a muon from the direction of the defect. The R axis denotes the position corresponding to the potential minimum of the metal matrix.

If there are a large number of minima near the defect, then the temperature dependence $\lambda(T)$ becomes more complicated.

From our point of view, a quantitative theoretical description of muon spin relaxation in a metal with defects in the case $\tau_1 \gtrsim \sigma_{tr}^{-1}$ is possible only by mathematical simulation, including a calculation of the energy of the interstitial sites around a defect and the muon spin relaxation rate in them, as well as a simulation of the motion of a muon in a metal with defects.

At high concentrations, where $\tau_1 \ll \sigma_{tr}^{-1}$, the function $\lambda(T)$ shown in Fig. 2 has been observed experimentally for the case $T_1 < T_0$. As has previously been stated, τ_1 can depend strongly on the temperature, and the condition $\tau_1 \ll \sigma_{tr}^{-1}$ can be violated for $T < T_1 < T_0$.

5. ANALYSIS OF EXPERIMENTAL DATA

In this Section we shall analyze the experimental data on μSR in metals and show that essentially all the data can be interpreted consistently within the framework of a unified model that explains the observed muon spin relaxation by the capture of the muon in traps.

5.1. Niobium

The muon spin relaxation in niobium has been the subject of many investigations.[28,29,35–41] The dependence of the observed relaxation rate on the concentration and kind of impurities has led to the conclusion that the muon spin relaxation in niobium (and also in a number of other metals except copper) is due to the presence of traps.[42] Modern data on the value of ε_0 for hydrogen in niobium[3,4] wholly support this conclusion.

FIG. 4. Muon spin relaxation rate vs the temperature when there are two types of bound states (a and b in Fig. 3) separated by a potential barrier.

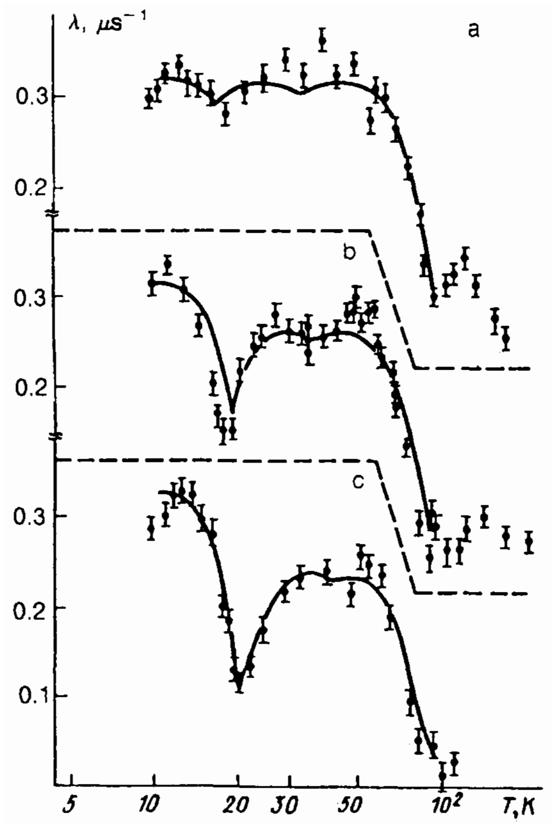

FIG. 5. Muon spin relaxation rate vs the temperature in niobium.[37] a) 3700 ppm of N, O, C. b) Less than 60 ppm of N, O, C. c) 10–20 ppm N, O, C.

The temperature dependence of the muon spin relaxation rate is shown in Figs. 5 and 6.

A characteristic feature of niobium is the presence of a minimum in $\lambda(T)$ in the vicinity of 20 K. When there is a large concentration of impurities this minimum vanishes and $\lambda(T)$ takes the form shown in Fig. 2 (curve *1*).

In principle, the presence of this minimum can be explained in two ways. First, one can assume that in the region of 20 K there is a maximum in τ_1, with $\tau_1^{\max} \gtrsim \sigma_{\mathrm{tr}}^{-1}$. Second, one can assume that there are two kinds of traps of different depth. The high- and the low-temperature parts of the plateau correspond to the capture of a muon in the trap with a large and small binding energy, respectively. The minimum of $\lambda(T)$ is due to the presence of the potential barrier around the deeper trap. For $T \sim 20$ K the muon cannot overcome this barrier but falls into the deep trap, while the shallower trap, even though it captures a muon, the time τ_2 of residence in it is short in comparison with $\sigma_{\mathrm{tr}}^{-1}$, which also leads to a small value of λ; i.e., the situation depicted in Fig. 4 occurs, but the valley between the high- and the low-temperature plateau occupies a narrow temperature range.

To make a choice between these two hypotheses, Petzinger[43] carried out measurements in zero magnetic field and studied the asymptotic behavior of the relaxation function $G(t)$. If the muon falls into a trap and remains there during the entire time of observation, then the value of $G(t)$ tends to 1/3 as t increases. However, if the muon jumps from trap to trap, then $G(t)$ tends to zero as t increases. The measurements show that in the region of the plateau the muon remains in a trap during the entire measurement time, while for $T = 18.5$ K in the region where

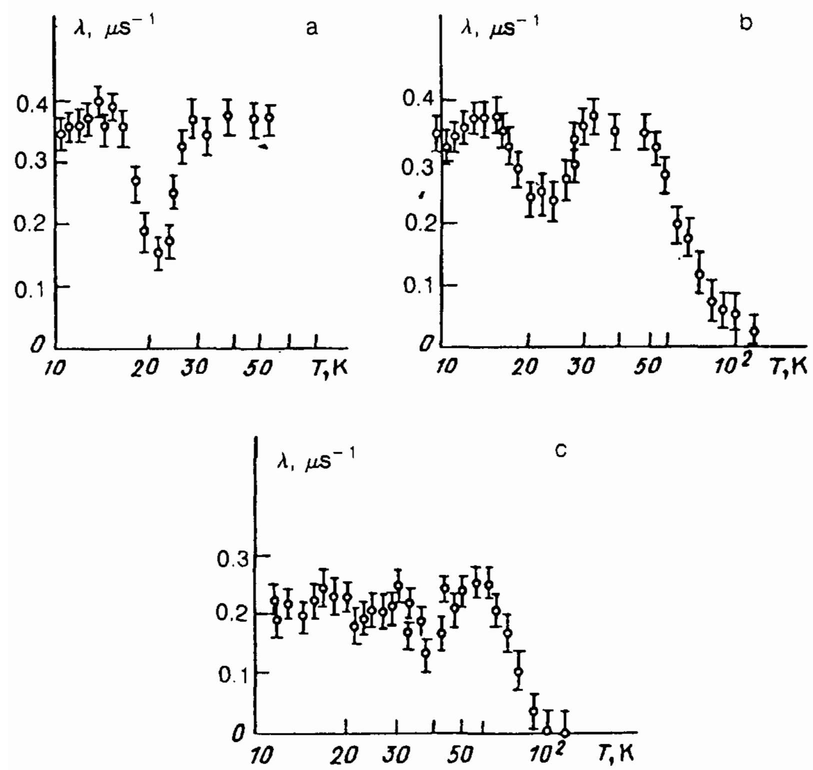

FIG. 6. Muon spin relaxation rate vs the temperature in niobium with oxygen impurity.[38]

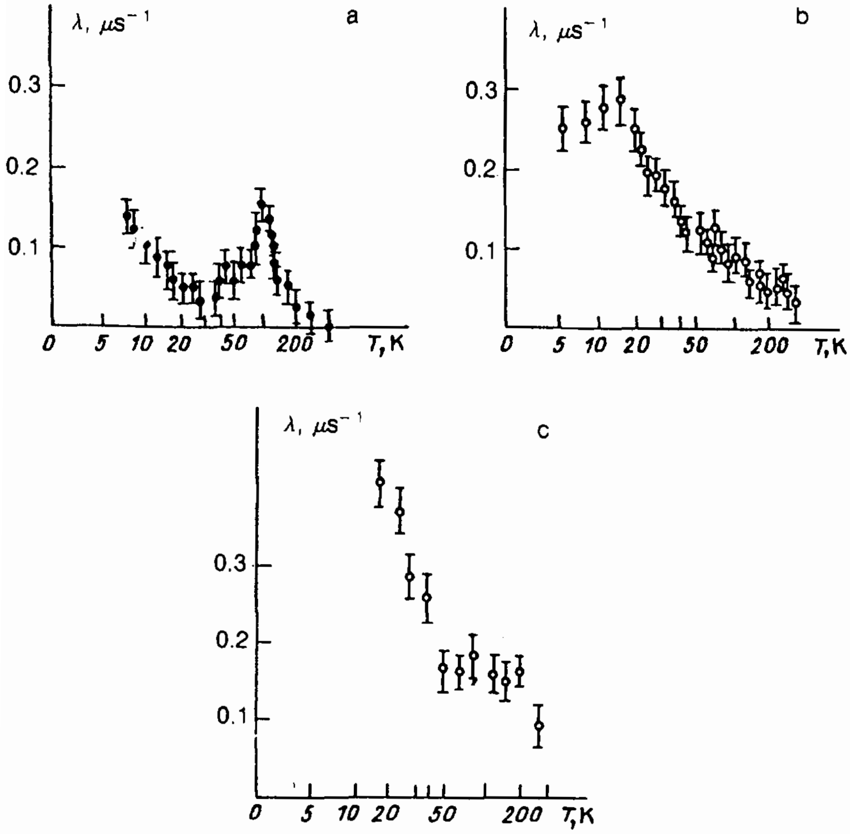

FIG. 7. Muon spin relaxation rate vs the temperature in vanadium[46] with various impurity concentrations. a) 15 ppm O; b) 500 ppm O; c) 0.5 at.% impurity.

the relaxation rate falls off with temperature, $G(t)$ tends to zero with increasing t.[40] Thus the decrease of λ after the low-temperature plateau is due to the escape of the muon from the trap (a reduction of the time τ_2) and not to an increase in the trapping time.

It was assumed in Ref. 41 that the presence of two kinds of traps is due to the presence of two types of impurities (N and Ta). However it is possible that because of the oscillatory nature of the interaction of the muon with a point defect both energy minima are created by the same defect.

The disappearance of the minimum in $\lambda(T)$ with increasing defect concentration is related both to the reduction in the time τ_1 (where $\tau_1(\tau_1 \propto x^{-1})$) and to the appearance of new types of energy minima caused by the action of two (or more) close-lying defects. The muon does not enter these minima by overcoming a high potential barrier, but the depth is sufficient that at $T \sim 20$ K the value of τ_2 would greatly exceed $\sigma_{\rm tr}^{-1}$.

In Ref. 36 it was shown that in the region of the high-temperature falloff of $\lambda(T)$ the value of $G(t)$ is well described by formula (16) under the assumption that

$$\tau_{\rm h}^{-1} = \nu_0 \exp(-E_{\rm a}/T),$$

where $\nu_0 = 10^{9.2 \pm 0.2}\ {\rm s}^{-1}$ and $E_{\rm a} = 50 \pm 2$ meV.

Using formula (30) for τ_2 we obtain the following estimate for the value of ε_0 in the tunneling of a muon from a deep minimum to a neighboring interstitial site: $\varepsilon_0 = 2$–3 K. The evidence that this transition is indeed quantum mechanical tunneling and not hopping over a barrier is the small value of ν_0. In the case of hopping over a barrier the value would be of the order of the local phonon frequency. However, if the muon escapes from a trap mainly by one-phonon processes, then for an estimate of ε_0 one must use formula (28).

5.2. Vanadium

The relaxation of muon spins in vanadium has been studied less thoroughly than in niobium. In particular, the measurements were carried out only with polycrystalline samples.[29,44–47]

The temperature dependence of the relaxation rate for vanadium containing different amounts of impurities[46] is shown in Fig. 7.

A characteristic feature of μSR in vanadium with a small concentration of defects is the presence of a sharp peak in the relaxation rate in the region 80–100 K. The absence of a plateau on the curve of $\lambda(T)$ and also the fact that the temperature that corresponds to the high-temperature decay of $\lambda(T)$ increases with increasing defect concentration indicates that the case $T_0 < T_1$ occurs in vanadium with a low concentration of defects.

The initial increase of λ with a reduction in temperature is due to the increase in the fraction of muons that are captured by traps, while the decay after the peak at 80–100 K is due to the fact that τ_1 increases with a decrease in the temperature because of the presence of a potential barrier in front of the trap.

The increase in λ as the temperature is lowered still

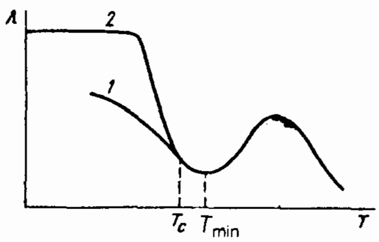

FIG. 8. Muon spin relaxation rate vs the temperature in aluminum. *1*) Normal metal; *2*) superconductor.

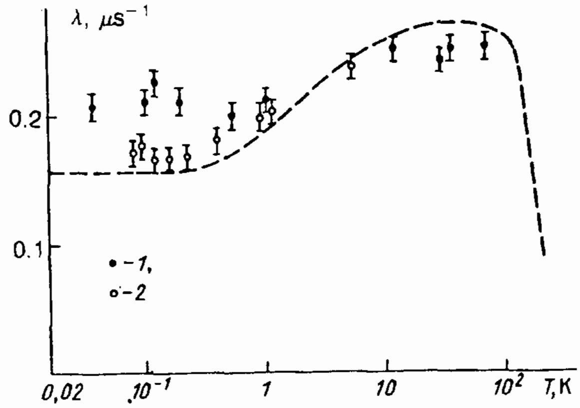

FIG. 9. Muon spin relaxation rate vs the temperature in copper before (*1*) and after (*2*) purification.[62]

further is due to the presence of shallower minima, as in the case of niobium. The "healing" of the minimum of $\lambda(T)$, which takes place at 30 K as the concentration of impurities increases,[46,47] is of the same nature as for niobium. The absence of a plateau on the curve of $\lambda(T)$ in the region of low temperatures indicates that $\tau_1(T) \gtrsim \sigma_{tr}^{-1}$ also in the range $T < 30$ K.

5.3. Aluminum

Aluminum is the metal that has been studied the most by μSR.[26,30,48–56] Its distinguishing feature is the absence of observable relaxation in the pure metal. This is due both to the high purity of the samples and the shallower energy minima created by the impurities in aluminum.

A characteristic curve of $\lambda(T)$ in aluminum with a small amount of Ag, Li, Mg, and Mn impurities[52] is shown in Fig. 8. It is similar to that for vanadium, i.e., in aluminum we also have the case $T_0 < T_1$. As the concentration of defects increases the relaxation rate increases and $\lambda(T)$ takes on the shape shown in Fig. 2 (curve *1*).[48,50,52]

The minimum on the curve of $\lambda(t)$ in the temperature region $T_{min} = 2$–4 K, as for vanadium, is related to the presence of two types of energy minima of different depths. Since $\lambda(T) = 0$ in pure aluminum, we can state with confidence that both types of minima are created by the same defect.

The fact that the minima in which the muon is located at temperatures above and below T_{min} are of a different nature is confirmed by the difference in the electric field gradient acting on the muon in a trap,[30] which is usually interpreted as a transition of a muon from a tetrahedral interstitial site to an octahedral site,[30,31] but it also might be related to the fact that the shallower minimum is located farther from the defect that acts as the trap.[30]

That the temperature dependence $\lambda(T)$ for $T < T_{min}$ is determined by the temperature dependence of τ_1 (see formula (45)) is proved by μSR experiments carried out in a zero magnetic field in superconducting aluminum.[55,56] The transition to the superconducting state at $T = T_c$ decreases the value of τ_1, since in the superconducting phase both the renormalized value of ε_0 and the number of electronic excitations are decreased, which leads to an increase in the mean free time of a muon (formula (7)). As a result, τ_1 becomes smaller than σ_{tr}^{-1} in the superconducting phase and $\lambda(T)$ assumes a constant value for $T < T_c$ (Fig. 8).

However, a comparison of $\tau_1(T)$ with the predictions of the theory for the diffusion coefficient in an ideal crystal does not, in our opinion, either confirm or refute the latter prediction, since the probability of capture of a μSR when it encounters a defect also depends on T, which leads to an exponential increase of τ_1 when there is a potential barrier in front of the trap. Therefore from the dependence $\tau_1(T)$ it is not possible to draw any direct conclusions about the temperature dependence of the diffusion coefficient of a muon in a pure metal.

5.4. Copper

The relaxation of the spin of a muon in copper has been studied in Refs. 23, 24, 50, and 57–64. While in the case of high concentrations the curve of $\lambda(T)$ is described by the curve shown in Fig. 2, in pure copper below $T = 2$ K we find that λ falls off with increasing temperature, and for $T < 0.5$ K there is a low-temperature plateau in $\lambda(T)$.[50,60,62] Such a curve is shown in Fig. 9.

Ordinarily this dependence is interpreted as the diffusion of a muon in the pure material without any traps. We believe that there are a number of insurmountable difficulties associated with this interpretation.

1. To explain the low rate of transition from interstitial site to site it is necessary, as is shown below, to assume that in copper $\varepsilon_0 \lesssim 10^{-3}$ K, i.e., many orders of magnitude smaller than in other metals.

2. The decay of $\lambda(T)$, which, according to experiment is exponential in the region of 100 K (Refs. 57, 29), is interpreted as a manifestation of incoherent diffusion due to interaction with phonons. In this case

$$\tau_h^{-1} = \nu_0 \exp(-E_a/T).$$

However, the temperature dependence for τ_h is exponential for $T > \Theta$ (Refs. 8, 12), and the Debye temperature of copper is $\Theta_{Cu} = 315$ K. An exponential dependence is also observed at $T \sim 100$ K.

3. The falloff of $\lambda(T)$ with a reduction in the temperature below 2 K is explained by the appearance of coherent

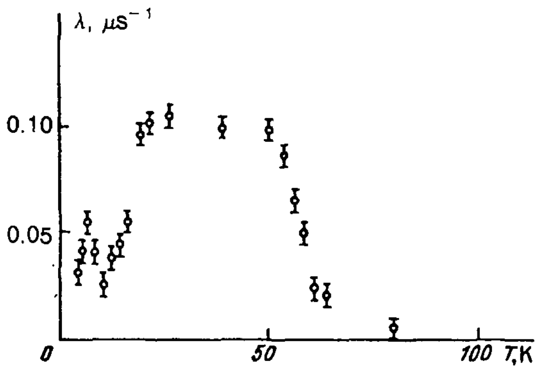

FIG. 10. Muon spin relaxation rate vs the temperature in tantalum.[39]

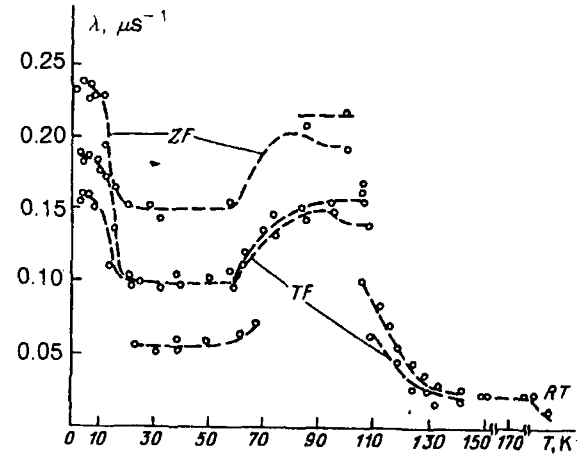

FIG. 11. Muon spin relaxation rate vs the temperature in bismuth in zero field (ZF) and a transverse magnetic field (TF) for various orientations of the sample;[69] RT—at room temperature.

diffusion. The rate of this diffusion increases as the temperature decreases. However, it remains unclear what causes the low-temperature plateau at $T<0.5$ K.

An alternate explanation, based on the assumption that the observed relaxation rate is due to traps, removes the first two objections. It is assumed that, as in the case of niobium, the observed hopping rate is τ_2^{-1}, and, using the data of Refs. 57 and 29 for ν_0 and E_a ($\nu_0=40.7\pm3.8$ MHz and $E_a=48.4\pm1.5$ meV according to Ref. 57 and $\nu_0=44.7\pm10$ MHz and $E_a=53.4\pm3.6$ meV according to Ref. 29) we find from formula (30) that $\varepsilon_0=0.5$–1 K.

The decrease in $\lambda(T)$ for $T<2$ K as the temperature is lowered, as we assume, is analogous to the minimum in $\lambda(T)$ in niobium at $T\approx20$ K and has the same cause. A muon is unable in the time of observation to fall into a deep minimum, while the time τ_2 for the shallower minimum is comparable to σ_{tr}^{-1}. This is confirmed by the nature of the dependence $G(t)$ measured in zero magnetic field.[24,64] In the temperature range 30 K $<T<$ 100 K the value of $G(t)$ for large t tends to the value 1/3, which indicates the localization of the muon in a single interstitial site, while for $T<30$ K, $G(t)\to0$, which indicates transitions of the muon from site to site. The introduction of impurities removes the falloff of $\lambda(T)$ in copper as it does for the minimum of $\lambda(T)$ in niobium.[61]

If our interpretation is correct, then as the temperature is further reduced one should again see the static relaxation function, which for large t tends to the value 1/3. The question of the nature of the spin relaxation in copper requires further study.

5.5. Tantalum

There have been fewer studies of μSR for tantalum than for copper or aluminum.[29,39,45,65]

As is the case for copper, when there is a high concentration of impurities the curve of $\lambda(T)$ is like that shown in Fig. 2, while for pure tantalum it is the same as that shown in Fig. 10 (Ref. 39). The falloff of $\lambda(T)$ in the region of 10–20 K has not been studied thoroughly, but it seems entirely probable that its nature is like that of the minimum of $\lambda(T)$ for niobium. On the basis of the data $\nu_0=3\cdot10^9$ s^{-1} and $E_a=42$ meV from Ref. 65, obtained with an approximation to $G(t)$ by formula (16) in the region of 50 K, we can, as in the case of Nb and Cu, estimate the value of the tunneling matrix element ϵ_0, which turns out to be 4–5 K.

5.6. Bismuth

A number of studies have been devoted to μSR in bismuth.[61,66–69] The observed temperature dependence of the relaxation rate is shown in Fig. 11. It is characterized by the presence of two plateaus at $T<10$ K and at $90<T<100$ K.[67] These sections of the curve correspond to a muon that is quickly localized in a trap and remains there during the entire measurement time.

As in the case of niobium, the decrease in the relaxation rate in the region $20<T80$ K is due to a) the presence of a potential barrier around the deepest energy minimum; b) insufficiently high binding energy in the shallow minimum.

The difference in the observed electric field gradient for temperatures that correspond to the low-temperature and the high-temperature plateau is due to the difference in the distance between the interstitial site in which the muon is localized and the point defect—the trap. As in the case of niobium, doping causes the dip in the curve of $\lambda(T)$ to disappear.[61] Since bismuth is a semimetal, and in it the value of $N(0)$ and consequently the value of g are small, the time t_2 for the release of a muon from the shallower minimum is due to one-phonon processes (formula (28)), and the release from the deep minimum is most likely to occur by means of surmounting a barrier, as is indicated by the large values $\nu_0=1.44\cdot10^{11}$ Hz and $E_a=128$ meV, obtained with the approximation for $G(t)$ in the region 100–200 K by formula (16), with $\tau_h^{-1}=\nu_0\exp(-E_a/T)$ (Refs. 69 and 67).

6. CONCLUSIONS

We have shown that the experimentally observed muon spin relaxation in metals (or at least in most metals) results from the muon being captured in a trap, which can be any point defect or extended defect in the crystal lattice.

Since the mutual position of the muon and the trap is an important factor that has a large influence on the muon spin relaxation rate, to obtain quantitative information on the local magnetic fields and on the quantum mechanical diffusion of the muon in a metal it is necessary to:

1. Carry out μSR investigations in ultrapure metals containing a controlled concentration of well-defined impurities in order to study the temperature and concentration dependences of the spin relaxation rate.

2. Study these samples in a zero and/or longitudinal magnetic field in order to determine from the dependence $G(t)$ in what temperature range the muon remains in the trap during the entire observation time.

3. Distinguish the contribution of the electrons to the rate of capture of muons by traps by comparing the temperature dependence of the muon spin relaxation rate in metals in the normal and superconducting phases.

4. Carry out a numerical simulation of the muon spin relaxation in a metal with defects starting from the calculated potential of the interaction between a muon and a defect and the energy distribution created by the muon among the interstitial sites.

5. Determine by numerical simulation the temperature dependence of the probability of capture of a muon by a trap when the muon is located at the boundary of the region of strong static distortion of the energy levels in the interstitial sites, and determine the temperature dependence of the diffusion coefficient in the pure crystal from the observed data for $\tau_1(T)$.

6. Determine which of the energy minima that serve as traps in the capture of a muon in niobium by impurities of oxygen and nitrogen correspond to a two-level system and compare the data with results of experimental investigations of hydrogen in niobium.[3,4]

[1] E. Karlsson, Phys. Rep. **82**, 272 (1982).
[2] S. F. J. Cox, J. Phys. C. **20**, 3187 (1987).
[3] K. Neumaier, D. Steinbinder, H. Wipf *et al.*, Z. Phys. B **76**, 359 (1989).
[4] H. Morr, A. Muller, G. Weiss *et al.*, Phys. Rev. Lett. **63**, 2084 (1989).
[5] A. I. Morozov, Zh. Eksp. Teor. Fiz. **77**, 1471 (1979) [Sov. Phys. JETP **50**, 768 (1979)].
[6] A. I. Morosov and A. S. Sigov, Solid State Commun. **53**, 31 (1985).
[7] J. Jäckle and K. W. Kehr, J. Phys. F **13**, 753 (1983).
[8] J. Kondo, Physica B+C **126**, 377 (1984).
[9] A. I. Morozov and A. S. Sigov, Fiz. Nizk. Temp. **13**, 606 (1987) [Sov. J. Low Temp. Phys. **13**, 341 (1987)].
[10] A. F. Andreev and I. M. Lifshitz, Zh. Eksp. Teor. Fiz. **56**, 2057 (1969) [Sov. Phys. JETP **29**, 1107 (1969)].
[11] A. F. Andreev, Usp. Fiz. Nauk **118**, 251 (1976) [Sov. Phys. Usp. **19**, 137 (1976)].
[12] P. S. Zyryanov and N. I. Klinger, *Quantum Theory of Electron Transport Phenomena in Crystalline Semiconductors* [in Russian], Nauka, Moscow (1976).
[13] A. I. Morosov and A. S. Sigov, J. Phys. Condens. Matter **2**, 505 (1990).
[14] E. Abrahams, *Electron Spin Resonance in Semiconductors* [Russian translation], IL, Moscow (1962).
[15] J. Kondo, *Hyperfine Interact.* **31**, 117 (1986).
[16] T. McMullen and E. Zaremba, Phys. Rev. B **18**, 3026 (1978).
[17] R. Kubo and T. Toyabe, *Magnetic Resonance and Relaxation*, North-Holland, Amsterdam (1967).
[18] A. I. Morozov and A. S. Sigov, Zh. Eksp. Teor. Fiz. **95**, 170 (1989) [Sov. Phys. JETP **68**, 97 (1989)].
[19] A. I. Morozov and A. S. Sigov, Solid State Commun. **67**, 841 (1988).
[20] J. Jäckle, L. Piche, W. Arnold, and S. Hunklinger, J. Non-Cryst. Solids **20**, 365 (1976).
[21] H. Sugimoto, J. Phys. Soc. Jpn. **55**, 1687 (1986).
[22] Yu. Kagan and N. V. Prokof'ev, Zh. Eksp. Teor. Fiz. **90**, 2176 (1986) [Sov. Phys. JETP **63**, 1276 (1986)].
[23] R. Kadono, J. Imazato, K. Nishiyama *et al.*, Phys. Lett. A **109**, 61 (1985).
[24] R. Kadono, J. Imazato, T. Matsuzaki *et al.*, Phys. Rev. B **39**, 23 (1989).
[25] K. W. Kehr, G. Honig, and D. Richter, Z. Phys. B **32**, 49 (1978).
[26] E. Sato, Y. Hatono, Y. Suzuki *et al.*, *Hyperfine Interact.* **17**, 203 (1984).
[27] A. A. Berzin, A. I. Morozov, and A. S. Sigov, Fiz. Tverd. Tela (Leningrad) **33**, 1161 (1991) [Sov. Phys. Solid State **33**, 602 (1991)].
[28] N. F. Gygax, A. Hintermann, W. Ruegg *et al.*, *Hyperfine Interact.* **17**, 177 (1984).
[29] H. Schilling, M. Camani, N. F. Gygax *et al.*, Hyperfine Interact. **8**, 675 (1981).
[30] O. Hartmann, E. Karlsson B. Lindgren *et al.*, *Hyperfine Interact.* **17**, 197 (1984).
[31] O. Hartmann, E. Karlsson, E. Wäckelgård *et al.*, Phys. Rev. B **37**, 4425 (1988).
[32] S. Kohn, J. A. Brown, R. H. Heffner *et al.*, *Hyperfine Interact.* **6**, 283 (1979).
[33] R. H. Heffner, *Hyperfine Interact.* **8**, 655 (1981).
[34] M. E. Schillaci, R. L. Hutson, R. H. Heffner *et al.*, *Hyperfine Interact.* **8**, 663 (1981).
[35] M. Borghini, T. O. Niinikoski, J. C. Soulié *et al.*, Phys. Rev. Lett. **40**, 1723 (1978).
[36] H. K. Birnbaum, M. Camani, A. T. Fiory *et al.*, Phys. Lett. A **65**, 435 (1978).
[37] T. O. Niinikoski, O. Hartmann, E. Karlsson *et al.*, *Hyperfine Interact.* **6**, 229 (1979).
[38] J. A. Brown, R. H. Heffner, M. Leon *et al.*, *Hyperfine Interact.* **6**, 223 (1979).
[39] H. Metz, H. Orth, and G. zu Putlitz, *Hyperfine Interact.* **6**, 271 (1979).
[40] C. Boekema, R. H. Heffner, R. L. Hutson *et al.*, Phys. Rev. B **26**, 2341 (1982).
[41] O. Hartmann, E. Karlsson, R. Wäppling *et al.*, Phys. Rev. B **27**, 1943 (1983).
[42] K. G. Petzinger, *Hyperfine Interact.* **8**, 639 (1981).
[43] K. G. Petzinger, Phys. Rev. A **75**, 225 (1980).
[44] A. T. Fiory, K. G. Lynn, D. M. Parkin *et al.*, Phys. Rev. Lett. **40**, 968 (1978).
[45] O. Hartmann, E. Karlsson, O. Norlin *et al.*, *Hyperfine Interact.* **6**, 237 (1978).
[46] R. H. Heffner, J. A. Brown, R. L. Mutson *et al.*, *Hyperfine Interact.* **4**, 824 (1978).
[47] V. G. Grebennik, I. I. Gurevich, V. A. Zhukov *et al.*, Zh. Eksp. Teor. Fiz. **80**, 298 (1981) [Sov. Phys. JETP **53**, 151 (1981)].
[48] W. J. Kossler, A. T. Fiory, W. F. Lankford *et al.*, Phys. Rev. Lett. **41**, 1558 (1978).
[49] W. J. Kossler, A. T. Fiory, W. F. Lankford *et al.*, *Hyperfine Interact.* **6**, 295 (1979).
[50] O. Hartmann, E. Karlsson, L. O. Norlin *et al.*, Phys. Rev. Lett. **44**, 337 (1980).
[51] J. H. Brewer, E. Koster, A. Schenk *et al.*, *Hyperfine Interact.* **8**, 671 (1981).
[52] K. W. Kehr, D. Richter, J. M. Welter *et al.*, Phys. Rev. B **26**, 567 (1982).
[53] T. Hatono, Y. Suzuki, M. Doyama *et al.*, *Hyperfine Interact.* **17**, 221 (1984).
[54] B. Hitti, W. J. Kossler, and J. R. Kempton, *Hyperfine Interact.* **31**, 211 (1986).
[55] O. Hartmann, E. Karlsson, S. Harris *et al.*, Phys. Lett. A **142**, 504 (1989).
[56] R. Kadono, R. F. Keift, S. R. Kreitzman *et al.*, *Hyperfine Interact.* **64**, 737 (1990).

[57] I. I. Gurevich, E. A. Meleshko, I. A. Muratova *et al.*, Phys. Lett. A **40**, 143 (1972).
[58] M. Camani, D. G. Fleming, F. N. Gygax *et al.*, *Hyperfine Interact.* **6**, 265 (1979).
[59] O. Hartmann, L. O. Norlin, A. Yaouanc *et al.*, *Hyperfine Interact.* **8**, 533 (1981).
[60] J. Chappert, A. Yaouanc, O. Hartmann *et al.*, Solid State Commun. **44**, 13 (1982).
[61] S. G. Barxov, A. L. Getalov, V. G. Grebinnik *et al.*, Zh. Eksp. Teor. Fiz. **85**, 341 (1983) [Zh. Eksp. Teor. Fiz. **58**, 198 (1983)].
[62] J.-M. Welter, D. Richter, R. Hempelmann *et al.*, Z. Phys. B **52**, 303 (1983).
[63] R. Kadono, J. Imazato, K. Nishiyama *et al.*, *Hyperfine Interact.* **17**, 109 (1984).
[64] G. M. Luke, J. H. Brewer, S. R. Kreitzman *et al.*, Phys. Rev. B **43**, 3284 (1991).
[65] H. Shilling, M. Camani, N. F. Gygax *et al.*, Phys. Lett. A **67**, 231 (1978).
[66] V. G. Grebinnik, I. I. Gurevich, V. A. Zhukov *et al.* Pis'ma Zh. Eksp. Teor. Fiz. **25**, 322 (1977) [JETP Lett. **25**, 298 (1977)].
[67] D. Baumann, F. N. Gygax, E. Lippelt *et al.*, *Hyperfine Interact.* **31**, 53 (1986).
[68] R. Kadono, K. Nishiyama, K. Nagamine *et al.*, Phys. Lett. A **132**, 195 (1988).
[69] F. N. Gygax, B. Hitti, E. Lippelt *et al.*, Z. Phys. B **71**, 473 (1988).

Translated by J. R. Anderson