DIPOLE INTERACTIONS AND TRAPPING EFFECTS OF POSITIVE
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INTRODUCTION

The use of positive muons (μ^+) as an experimental probe of lattice defects, in analogy with the use of positrons for the same purpose, has been previously suggested.^{1,2,3,4} There are several aspects involved with the interpretation of the experimental data that are poorly understood. After a μ^+ is thermalized in a solid, its subsequent behavior can include trapping at a vacancy or interstitial site, or diffusing by a classical or quantum mechanism between various equivalent or non-equivalent lattice sites.^{5,6,7} The experimentally determined quantity is the depolarization rate of a polarized positive muon. For most metals the depolarization rate is determined by the crystalline dipole field at the muon site. As an attempt to determine possible muon trapping locations from low temperature experimental data, we have studied a simple model that specifically treats the dipole-dipole interactions between the μ^+ and the crystalline field.

In this paper we shall present the results of our calculations for a single muon trapped at various lattice sites in an external magnetic field. As the direction of the magnetic field is changed, our results show a large variation of the local field experienced by a muon at the octahedral (o-sites) and tetrahedral (t-sites) symmetry lattice interstitial sites. These results show that a careful measurement of the μ^+ depolarization rate for various external magnetic field orientations would indicate a preferential position for the trapped particle. At this time analysis of the experimental data⁷ does not present a clear interpretation for the determination of the μ^+ site. In what follows we shall outline our calculational procedure and present the results, including an estimate of the effects of lattice distortion on the μ^+ depolarization rate when the muon is localized.

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The details of measuring μ^+ depolarization may be found in Ref. 4. The time dependent damping of the μ^+ precession amplitude can be approximated by a Gaussian line shape, in which case a knowledge of the second moment of the frequency provides a description for the line width. In this calculation we are ignoring the higher order moments, since inclusion of these moments only changes the predicted curve by giving the Gaussian line shape a flatter top. Van Vleck's⁸ calculation of the second moment of the frequency, for unlike spins with dipole interactions can be applied to the case of a single muon, with spin I_μ and gyromagnetic ratio γ_μ , interacting with a crystal of like spins I and gyromagnetic ratios γ_I . The decay of the transverse polarization $P(t)$ is then proportional to $\exp(-\Omega^2 t^2)$ where

$$\Omega^2 = \frac{1}{6} I(I+1) \hbar^2 \gamma_I^2 \gamma_\mu^2 T_n, \quad (1)$$

$$T_n = \sum_{i=1}^n \left\{ \frac{(1 - 3 \cos^2 \theta_i)}{|\vec{r}_i - \vec{r}_\mu|^3} \right\}^2. \quad (2)$$

$\hbar$ is Planck's constant and θ_i is the angle between the external magnetic field $\vec{H}$ and $(\vec{r}_i - \vec{r}_\mu)$ where $\vec{r}_i$ is the position of the i th nucleus and $\vec{r}_\mu$ is the position of the muon. We have calculated T_n for fcc and bcc lattices for $\vec{r}_\mu$ at a lattice substitutional site, at an o-site, and at a t-site. $\vec{H}$ was varied continuously from the (100) to the (110) direction, the (110) to the (111) direction, and the (111) to the (100) direction. The results for the case of no lattice distortion are shown in Figs. 1 and 2 for the fcc and bcc lattices, respectively. The numbers in parenthesis in Fig. 1 are the neutron irradiation levels in neutrons/cm² for specific Cu samples. In Fig. 2 the o-site and t-site values plotted are the average of their respective nonequivalent site values that result from specifying a magnetic field direction. The summations in Eq. (2) were calculated with a convergence accuracy of greater than 0.01%.

Experimental data for single crystal Cu,⁷ polycrystalline Cu,⁵ and polycrystalline Al⁶ are shown in Fig. 1. The low temperature experimental values of the depolarization rate were used in Eq. (1) and the lattice sum T_n was determined. For the polycrystalline samples the data is plotted near the powder average⁹ results. With the exception of the single crystal Cu data point at (100), one might conclude that the muon was sitting at a t-site. The result for polycrystalline Cu also leads one to the same conclusion. This result seems to be in disagreement with the recent work at SIN where they conclude that the μ^+ is only residing at the o-site in Cu.¹⁰ The addition of the (100) point makes a simple interpretation more difficult. In Al, the data on polycrystalline samples and single crystal samples with an undetermined orientation⁷ suggest that the μ^+ prefers a substitutional lattice site, and because no depolarization was observed for temperatures up to 300 K, the μ^+ may be strongly bound to that site. This interpretation is consistent with the calculations of Popovich and Stott² where they find a binding energy of 1.2 eV for a hydrogen ion in a vacancy in aluminum. Trapping at a vacancy in Al requires that the μ^+ be able to find a vacancy during the latter portion of its thermalization process when the kinetic energy of the muon is less than the binding energy to a vacancy, or be able to find a vacancy as it diffuses through the lattice. Another possible interpretation of the Al results is that the muon is trapped at a dislocation or a kink in a dislocation. One would expect that the crystalline dipole field at a dislocation would be more nearly that of a vacancy than an interstitial site and hence the depolarization rate would be similar to trapping at a vacancy.

We have made estimates of the effect of lattice distortion by assuming a radial displacement of the atoms around the μ^+ . The displacement, Δr , of an atom at a distance r from the muon was taken to be

$$\Delta r = \delta/r^m$$

where δ may be positive or negative and m in the range of 2 to 4. The change in the depolarization rate is given by

$$\frac{\Delta\Omega}{\Omega} = \left(\sqrt{T'_n} - \sqrt{T_n} \right) / \sqrt{T_n} ,$$

where T'_n and T_n are calculated from Eq. (2) with the primed quantity indicating the distorted case. For the t-sites and o-sites at $\vec{H} = (100)$ and $\vec{H} = (111)$, the large differences between the calculated Ω 's decreased. When $\Delta r/r$ for nearest neighbors to the μ^+ was approximately +0.05, $\Delta\Omega/\Omega \cong -0.13$ ($m=2$; $\vec{H} = (100)$) for the t-site and $\Delta\Omega/\Omega \cong -0.02$ for the o-site. For all values of $\Delta r/r$, the ratios for the frequency changes for the two sites were approximately a factor of 10. The same results were obtained at $\vec{H} = (111)$ except that the relative rates of the two sites were reversed and the frequency calculated for the o-site decreased more rapidly than that of the t-site. If one assumes that for the substitutional site the lattice relaxes in towards the vacancy, then a $\Delta r/r = -0.05$ produces a $\Delta\Omega/\Omega = +0.14$. As expected the net effect of the inclusion of lattice distortion is to reduce the difference in depolarization rates between the possible μ^+ positions, for both fcc and bcc metals. Perhaps a more meaningful measurement for determining the μ^+ site other than the magnitude of the depolarization rate would be the derivative of the polarization rate with respect to changes in the field direction. For some crystal orientations the sign of the derivative would suffice.

The error bars plotted in Fig. 1 are the statistical error only resulting from fitting the raw experimental data to a Gaussian curve. Estimates of systematic experimental error owing to sample alignment, magnetic field inhomogeneities, and variations in the incident beam polarization could significantly increase the magnitude of the error bars. Better experimental data is needed before one can make a conclusive determination of the μ^+ trapping site. A full theoretical treatment of the nonlinear screening of the electron gas in the vicinity of the muon and a calculation of that potential for the trapping of muons at interstitial and vacancy sites should be performed.

References

1. W. J. Kossler, Topical Meeting on Intermediate Energy Physics, Zurich, Switzerland, April 4-13, 1973 (Report No. CERN 74-8, 1974).
2. Z. D. Popovic and M. J. Stott, Phys. Rev. Lett. 33, 1164 (1974).
3. A. Seeger, Phys. Lett. 53A, 324 (1975).
4. A. Schenck in Nuclear and Particle Physics at Intermediate Energies, edited by J. B. Warren (Plenum Press, 1976).
5. V. G. Grebinnik, I. I. Gurevich, V. A. Zhukov, A. P. Manych, E. A. Meleshko, I. A. Muratova, B. A. Nikol'skii, V. I. Selvonov, and V. A. Suetin, Sov. Phys. - JETP, 41, 777 (1976).
6. I. I. Gurevich, E. A. Meleshko, I. A. Muratova, B. A. Nikol'sky, V. S. Roganov, V. I. Selivanov, and B. V. Sokolov, Phys. Lett. 40A, 143 (1972).
7. W. B. Gauster, A. T. Fiory, K. G. Lynn, W. J. Kossler, and D. M. Parkin - this conference.
8. J. H. Van Vleck, Phys. Rev. 74, 1168 (1948).
9. A. Abragam, The Principles of Nuclear Magnetism (Oxford University Press, 1961).
10. A. Schenck, private communication.

Figures

- Fig. 1. T_n as calculated from Eq. (2) as a function of the magnetic field orientation for a fcc lattice. The solid line is for the o-site, the dashed line is for the t-site, and the dotted line is for the substitutional site. Powder average values are indicated by $\langle \rangle$. The error bars do not include possible systematic experimental error. The numbers in parenthesis are prior neutron irradiation levels in neutrons/cm².
- Fig. 2. T_n as calculated from Eq. (2) as a function of the magnetic field orientation for a bcc lattice. The solid line is for the o-site, the dashed line is for the t-site and the dotted line is for the substitutional site. Powder average values are indicated by $\langle \rangle$.