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IN METALS AT LOW TEMPERATURE

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CONTRIBUTION TO THE THEORY OF POSITIVE MUON DIFFUSION
IN METALS AT LOW TEMPERATURE

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ABSTRACT

We study the temperature dependence of the μ^+ diffusion in a metal within the small polaron theory. The geometry of the strain field due to an impurity is shown to strongly influence the μ^+ diffusion properties. We reanalyzed part of the Al data.

Recently, detailed μ^+ SR experiments have been performed on Al and Al alloys.^[1] These experiments have shown that the μ^+ diffuses by a quantum tunneling between ground state levels of interstitial sites. The data indicate that the μ^+ can diffuse coherently or incoherently depending upon its distance from the impurities and the temperature.

In this short note we will give some recent developments concerning the diffusion theory. We will stress the importance of the strain field geometry and show that these recent developments possibly can explain the experimental data on Al.

^{*}Part of this work was done at the French Atomic Commission at Grenoble.

We first suppose that the μ^+ form a small polaron in a homogeneous metal. The μ^+ correlation time is approximately equal to the μ^+ mean time of stay, τ_s , at least in fcc lattices. τ_s can be expressed in terms of the on-site correlation function, $G_s(l, t/l, 0)$. If the μ^+ diffuses coherently we have [2]

$$G_s(l, t/l, 0) = \exp(-N\psi) \quad (1)$$

$$\psi = 4 \sum_{\gamma, l'} e^{-\beta \theta_{\gamma}} |\langle l, \gamma | \tilde{H}_s | \gamma, l' \rangle|^2 \int_{-\infty}^{\infty} \mathcal{P}(x) \sin(xt/2)/x^2 dx \quad (2)$$

where $\tilde{H}_s$ is the jumping part of the μ^+ -crystal Hamiltonian. It describes the μ^+ tunneling. It is renormalized by the phonons. $\mathcal{P}(x)$ is the distribution of energy levels between two adjacent interstitial sites. It takes into account the distributions due to the phonons, the strain field, etc. From Eqs. (1) and (2) it can be shown that the coherent diffusion cannot be measured directly in Al. [2] It can only be seen indirectly.

We have analyzed the incoherent diffusion mode of the μ^+ . [2,3] The main point is that the interstitial sites between which the μ^+ diffuses cannot have the same symmetry at low temperature. In order to explain the data obtained in fcc crystals at low temperature, it has been suggested that a dynamical mechanism can possibly break the symmetry. [4]

We would like to mention the consequence of the particular geometry of the long-range part of the strain field due to an impurity. [2] This analysis has been performed for diffusion between octahedral sites in a fcc crystal but the results should be general. When the μ^+ diffuses incoherently it is always attracted by the impurity. This property does not depend on the parameters describing the μ^+ -impurity interaction. There are on the average three nearest neighbor interstitial sites to the μ^+ site

which have the same energy as the μ^+ site. This property has an important consequence when the μ^+ diffuses coherently. Because there are on the average $1/4$ of the nearest sites which are unperturbed by the strain field, this field cannot possibly localize the μ^+ . This property is well-known for electrons in disorder systems.^[5] We would like to point out that $1/4$ is a lower limit because if a site is just a little disturbed by the strain field, it will be counted as a site favorable for coherent diffusion.

A detailed analysis of the Al data^[1] at low temperature ($T \lesssim 1K$) shows that the μ^+ diffuses coherently in the purest part of the sample.^[1] This diffusion is capture-controlled^[2] and at 1K the capture radius is $\sim 4 \text{ \AA}$. This small value shows that the μ^+ is localized by the short-range part of the μ^+ -impurity interaction.

The μ^+ is probably a small polaron in Al. But we notice that if the μ^+ is not a small polaron, it can diffuse coherently in a metal by a one phonon process the temperature dependence of which is very slight.^[2]

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