

Nuclear spin-lattice relaxation time T_1 and bare state density on the Fermi surface $N(0)$ in Nb-Ti alloys

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The method of pulsed NMR on Nb^{93} nuclei was used to measure the spin-lattice relaxation time T_1 in Nb-Ti alloys. The data on T_1 were used to calculate the bare density of states on the Fermi surface $N(0)$ as a function of the Ti content. It was observed that $N(0)$ has a maximum at ~ 25 at. % Ti.

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Much progress was made recently in the theory of spin-lattice relaxation of transition metals.^[1] It follows from the theory of spin-lattice relaxation that T_1 is directly proportional to $N^2(0)$, which is the square of the bare density of states on the Fermi surface (the density of states for a gas of noninteracting electrons). As shown in^[2], the spin-lattice relaxation contains precisely $N(0)$, and not the state density determined from data on the electronic specific heat, $N_v(0)$, which is larger than $N(0)$ because of the electron-phonon and Coulomb interactions. Thus, experiments on spin-lattice relaxation make it possible to determine $N(0)$, and a comparison of $N(0)$ with $N_v(0)$ yields the parameters of the electron-phonon and electron-electron interactions. In this study we measured T_1 in Nb-Ti alloys and determined $N(0)$ and its dependence on the titanium content in the alloys.

The investigated alloys were fused by an induction method. The ingots were homogenized at 1500°C for 10 hours, and then quenched in water from 1100°C. The composition of the investigated alloys was monitored by chemical analysis. The samples for the investigations were powders with dimensions not exceeding 40 μ . The spin-lattice time was determined at 77°K in a field 18.7 kOe with a "Bruecker" NMR pulsed spectrometer. Various combinations and sequences of pulses were used ($180^\circ \tau 90^\circ; \pi 90^\circ \tau 90^\circ; 90^\circ \tau 90^\circ + 180^\circ$, etc). All yielded for T_1 values that agreed within 7%.

Figure 1 shows the concentration dependence of $(T_1 T)^{-1}(c)$, where T is the temperature of the experiment and c is the titanium concentration in at. %. The value of T_1 measured by us in niobium coincides exactly with the data of others.^[3] It is seen from Fig. 1 that $(T_1 T)^{-1}$ has a maximum for compositions that contain ~ 25 at. % Ti. We note that when zirconium is added to niobium, $(T_1 T)^{-1}$ also has a maximum at ~ 30 at. % of zirconium.^[3] The presence of maxima of $(T_1 T)^{-1}$ in Nb-Ti and Nb-Zr alloys at a close concentration of Ti and Zr in niobium is not surprising, since these alloys correspond approximately to one and the same electron concentration $e/a \sim 4.75-4.70$.

In the tight-binding approximation, for a cubic crystal, the total nuclear spin-lattice relaxation rate is expressed in analytic form as the sum of the relaxation rates due to three mechanisms:

$$\frac{1}{T_1} = \left(\frac{1}{T_1} \right)_{\text{con}} + \left(\frac{1}{T_1} \right)_{\text{pol}} + \left(\frac{1}{T_1} \right)_{\text{orb}}, \quad (1)$$

where the subscripts "con," "pol," and "orb" correspond to the contact hyperfine interaction, the interaction due to the polarization of the filled s shells, and the orbital interaction, respectively. The complete expression for the nuclear spin-lattice relaxation rate is

$$\frac{1}{T_1 T} = 4\pi\gamma_n^2 \hbar k_B [N(0)]^2 \{ [\rho H_{\text{con}}]^2 + [(1-\rho)h_{\text{pol}}]^2 + [(1-\rho)h_{\text{orb}}]^2 \} p^q, \quad (2)$$

In this expression, T is the temperature of the experiment, γ_n is the nuclear gyromagnetic ratio, k_B is the Boltzmann constant, $N(0)$ is the bare density of states on the Fermi surface for one direction of the spin, $\rho = N_s(0)/N(0)$ is the ratio of the s -electron state density $N_s(0)$ to the summary state density, H is the corresponding hyperfine field (hff) for a definite type of interaction, and the parameters q and p are expressed in terms of the degree f of the presence of the atomic functions Γ_5 on the Fermi surface. q and p as functions of f were calculated in^[1] and are given by

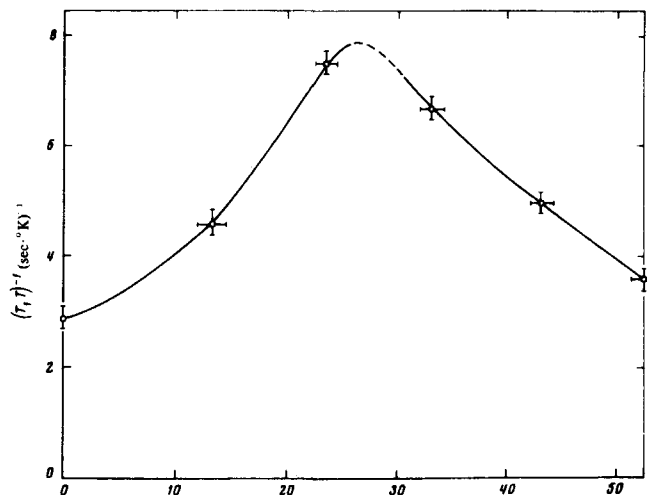


Fig. 1. Concentration dependence of the spin-lattice relaxation rate $(T_1 T)^{-1}$ in Nb-Ti alloys.

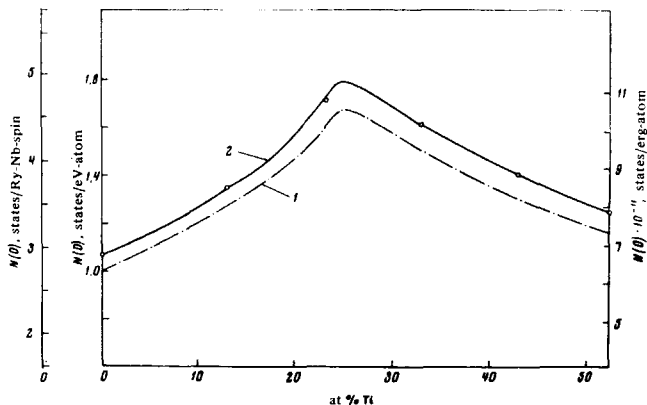


Fig. 2. Concentration dependence of the bare density of states $N(0)$ in Nb-Ti alloys: 1— $N(0)$ calculated for $H_{\text{orb}} = 0.285 \times 10^6$ Oe; 2— $N(0)$ calculated for $H_{\text{orb}} = 0.75 \times (0.285 \times 10^6)$ Oe.

$$q = \frac{1}{3} (f)^2 + \frac{1}{2} (1-f)^2, \quad (3)$$

$$p = \frac{2}{3} f(2 - \frac{5}{3} f).$$

The relaxations due to the dipole and quadrupole interactions are small and were not taken into account.^[1] The values of the hff due to various causes are known for niobium. We chose the same values of the hff as in^[4] for the calculation of T_1 of niobium. It is usually assumed that the wave functions of electrons with Fermi energy can be limited to atomic functions with orbital numbers $l=0$ and $l=2$, from which we have $N(0) = N_s(0) + N_d(0)$. However, the atomic functions $l=1$ can also contribute to the summary density of states $N(0)$. But the hff due to the p electrons is small in comparison with the hff from the s and d electrons.^[1] The contri-

bution of the p electrons to T_1 is therefore small, and we can neglect the contribution of these electrons to $N(0)$. The main contribution to $N(0)$ on the Fermi surface is made by the d electrons. Therefore a good approximation for ρ in niobium is $\rho = 0.1$.^[4] We assume here that ρ does not vary with composition, in analogy with the assumption made in the study^[5] of $(T_1 T)^{-1}$ in vanadium-based alloys with structure A15. The last parameter we need for the calculation of $N(0)$ is the relative weight f of the atomic functions of states of type Γ_5 on the Fermi surface. In accordance with the splitting of the atomic d levels in a cubic field into triply (Γ_5) and doubly (Γ_3) degenerate levels, we should choose $f = 0.6$. Since we are considering only alloys with bcc lattices, it follows that f is constant for all the alloys.

Figure 2 shows the concentration dependence of the bare density of states $N(0)$, calculated from formula (2). $N(0)$ has a maximum in the region of compositions ~ 25 at.% Ti. An analysis has shown that certain variations of the parameters ρ , H , and f in Eq. (2) do not change the form of the dependence of $N(0)$ on the composition, and the values of $N(0)$ change insignificantly. Thus, band calculations^[6] yielded $\rho \cong 0.06$. The calculated $N(0)$ for $\rho \cong 0.06$ barely differ from those shown in Fig. 2. It is seen from the figure that a 25% change of H_{orb} changes $N(0)$ by approximately 6%.

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