Two-Level System Constituted by Trapped Deuterium in Nb and Ta

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Two-Level System Constituted by Trapped Deuterium in Nb and Ta

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The two-level system (TLS) model is used to interpret the anelastic relaxation observed in the Nb-O(N)-D and Ta-O(N)-D systems at low temperature. In Ta there is clear evidence that the TLS interact mainly with the conduction electrons.

1. INTRODUCTION

In Nb and Ta interstitial hydrogen and deuterium are trapped by heavy interstitial impurities and give rise to effects at low temperature which are due to their tunneling among sites coordinated with the trapping centres |1-6|. The geometry of the tunnel system and the nature of the transitions of H(D) among the quantized levels is at present object of investigation. The present paper displays further evidence that a two-level system (TLS) model with transitions assisted by electrons explains many features observed in Nb and Ta at low temperature.

2. EXPERIMENTAL

The samples were polycrystalline circular plates of Nb (30 mm in diameter and 2.5 mm thick) containing 0.13 at% O and 0.015 at% N, and of Ta (36 mm in diameter and 1.4 mm thick) with 0.053 at% O and 0.016 at% N. Deuterium doping was carried out in the annealed samples by thermal treatments in appropriate gas atmospheres.

3. RESULTS AND DISCUSSION

The anelastic relaxation Q^{-1} as a function of temperature of Nb-O(N) doped with deuterium is composed of two thermally activated peaks placed, for a vibration frequency of 20 kHz, at 1.5 and 4 K |2|; in fig. 1 is shown only the peak at 4 K, which will be analyzed here. A similar spectrum is obtained in the H doped sample, with the peak temperature shifted to lower values |2|. The anelastic relaxation as a function of inverse temperature of the Ta-O(N) sample doped with 0.25 at% D at 7.5 and 30 kHz is presented in fig. 2.

In Nb the process giving rise to the peak at lower temperature has been detected with various experimental techniques and attributed to a TLS constituted by an O-H(D) complex with tunnel energy of about 2÷3 K for H and 0.24 K for D |1,3-6|. Because the theory of TLS is independent of the exact atomic configuration which tunnels |7|, it can be supposed that also the present higher temperature peak in Nb is due to a TLS arising from a different O-H(D) configuration or an O-2H(2D) complex |1|.

In the case of an O-H(D) complex it is supposed that H(D) is delocalized near the O(N) trap in two equivalent sites, which may differ in energy of Δ due to the elastic interactions with the other defects; the first two levels of the tunnel system are splitted of $E = (\Delta_0^2+\Delta^2)^{1/2}$, where Δ_0 is the matrix element of tunneling. The vibration of the sample changes E, giving rise to anelastic relaxation whose intensity is:

$$\delta(T) = \frac{nD^2}{4cE}\,\beta E\,\mathrm{sech}^2(\beta E/2)$$

where n is the volume concentration of TLS, $D = dE/d\varepsilon$ is the change of E with strain ε, c the elastic stiffness coupled to the TLS and $\beta = 1/kT$. The relaxation peak is given by the Debye formula:

$$Q^{-1}(T) = \delta(T)\,\frac{\omega\tau}{1+(\omega\tau)^2}$$

where ω is the angular frequency of vibration and $\tau(T)$ the relaxation time of the TLS; $\tau(T)$ depends on the type of interaction between the TLS and its environment, which can occur through phonons and through the conduction electrons.

The one-phonon contribution to the relaxation frequency is slowly varying with temperature, $\tau_{1ph}^{-1} \propto \coth(\beta E/2)$; it would give rise to peaks broader than those observed and therefore it will not be considered here.

The contribution from two-phonon transitions has a much stronger dependence on T, $\tau_{2ph}^{-1} \propto T^7$ in the high temperature limit, and therefore gives rise to narrow peaks. Higher order transitions should be relevant at higher temperature and will be neglected here.

Another type of interaction of the TLS with the crystal is through the conduction electrons. The temperature dependence of τ_{el}^{-1} is identical with the one-phonon relaxation:

$$\tau_{el}^{-1} = \frac{\pi}{4\hbar}\,|K_{\parallel}\, n(E_F)\,\Delta_0/E|^2\, E\coth(\beta E/2)$$

where $n(E_F)$ is the electron density of states at the Fermi level and $K_{\parallel}$ is the TLS-electron coupling.

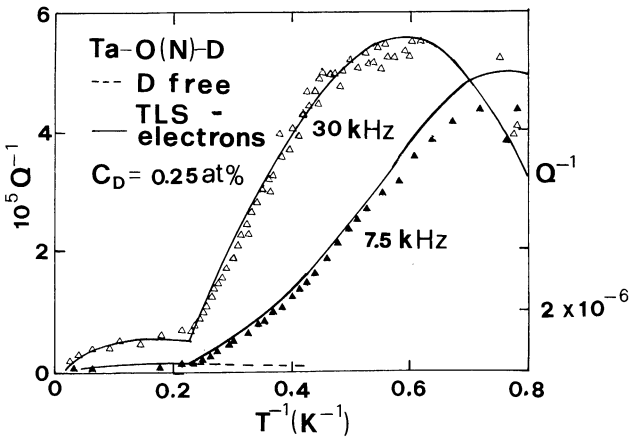

Fig. 1. Anelastic relaxation in Nb-O(N)-D at two vibration frequencies. Shown are also the best fits with two-phonon and electron interaction.

The relaxation rate drops when the metal becomes superconductor, because the number of free electrons able to interact with the TLS is reduced |8|. For E less than the BCS energy gap Δ_S the expression of the relaxation rate is approximately:

$$\tau_{el}^{-1} = \frac{\pi}{\hbar} |K_{\parallel} n(E_F) \Delta_0 / E|^2 [\beta(1+e^{\beta\Delta_s})]^{-1}$$

which is again strongly dependent on temperature.

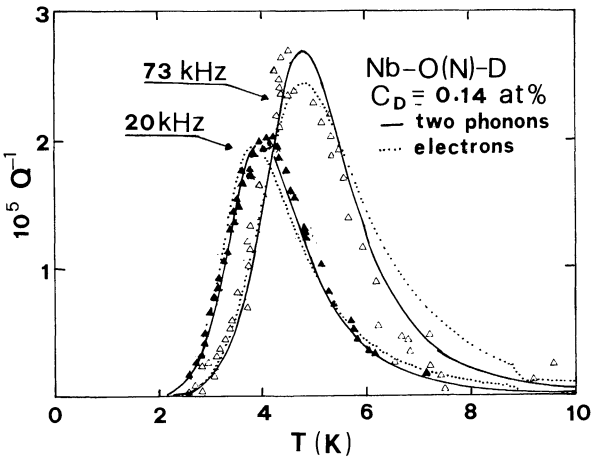

Fig. 2. Anelastic relaxation in Ta-O(N)-D at two vibration frequencies. The solid line represents the fit for the TLS-electron interaction.

In fig. 1 are shown the fits to the peak measured in Nb-O(N)-D obtained assuming electron or two-phonon interaction; they are nearly equivalent and in both cases $E \cong \Delta_0 \cong 10$ K is obtained for the tunnel energy; it is impossible from these fits to decide which of the mechanisms is predominant. A similar result is obtained in Nb-O(N)-H |2|, with nearly the same value of Δ_0; the absence of the isotope effect on Δ_0 is in disagreement with theory, which would predict a lower value of the tunnel energy for D than for H. For the coupling to the electrons $K_{\parallel} n(E_F)$, 1.3×10^{-2} and 3.1×10^{-3} is found for H and D respectively.

In the tantalum-deuterium system the relaxation curve extends itself in both the normal and superconducting regions, and has a discontinuity in the slope at the transition temperature T_c, suggesting that the relaxation is mainly governed by the electrons. Indeed, the analysis in terms of TLS interacting with the electrons, shown in fig. 2 as a continuous line, is satisfactory. Because deuteride formation occurred in the Ta sample, the large random strains due to precipitation give rise to an appreciable distribution of the asymmetry Δ, which was assumed to be a gaussian of width σ_Δ. From the fit the following values of the parameters of the TLS were obtained:

$\Delta_0 = 1$ K $K_{\parallel} n(E_F) = 1.7\times10^{-2}$ $\sigma_\Delta = 15$ K.

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