Knight Shift in the V_3Ga Compound at High Temperatures

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The temperature dependence of the Knight shift of both ^{51}V and ^{71}Ga in the V_3Ga compound has been measured over the entire range from 300 K to 1300 K. The results are discussed using a model based on the assumption that the core polarization contribution to the total Knight shift is the temperature dependent term.

Nuclear magnetic resonance studies have provided important information about the electronic properties of a wide variety of V_3X compounds [1, 2]. It has been found that the compounds with the highest superconducting transition temperature T_c show the greatest temperature coefficient of the Vanadium Knight shift $K_{^{51}V}$ in the non-superconducting state up to 400 K [1]. Therefore it is very interesting to ask how the various mechanics contribute to the hyperfine properties and how the temperature variation influences the system.

In the present work we report on Knight shift measurements in the high temperature range (300 – 1300 K) concerning the isotopes ^{51}V and ^{71}Ga in V_3Ga. Figure 1 shows the Knight shift $K_{^{51}V}$ as a function of temperature. As a reference sample for the determination of $K_{^{51}V}$ we used $V_3(SO_4)_3$. The average temperature coefficient α_1 of $K_{^{51}V}$ in V_3Ga for the range (300 – 1300 K) is $\alpha_1 = 5.5 \cdot 10^{-5}\,\%\,K^{-1}$. This value of α_1 is almost the same as the value of the temperature coefficient α_2 of $K_{^{51}V}$ in pure vanadium metal, $\alpha_2 = 4.5 \cdot 10^{-5}\,\%\,K^{-1}$, a value which was found for the same range (300 – 1300 K) in our earlier work [3]. Additionally, we found that $K_{^{51}V}$ in V_3Ga and in pure vanadium metal has almost the same value between 300 K and 1300 K. This is an indication that similar mechanisms are responsible for the hyperfine field at the ^{51}V position in both systems, V_3Ga and pure vanadium at high temperatures. As is reported in [1], the temperature coefficient of $K_{^{51}V}$ in V_3Ga amounts to $39 \cdot 10^{-5}\,\%\,K^{-1}$ in the range between T_c and 300 K, whereas the temperature coefficient of $K_{^{51}V}$ for pure vanadium amounts only to $1 \cdot 10^{-5}\,\%\,K^{-1}$ between T_c and 300 K. The experimental results for the Knight shift $K_{^{71}Ga}$ of ^{71}Ga in the V_3Ga compound for temperatures between 300 K and 1300 K are shown in Figure 2. For the determination of $K_{^{71}Ga}$ we used $GaCl_3$ as a reference sample. $K_{^{71}Ga}$ is negative over the entire temperature range and has between 300 K and 1300 K a temperature coefficient $\beta = 23 \cdot 10^{-5}\,\%\,K^{-1}$, whereas β shows between T_c and 300 K the large value of $170 \cdot 10^{-5}\,\%\,K^{-1}$.

A comparison between the results of our previous measurements on V_3Si [3] and those of the present work shows that the minority constituents X of the V_3X compounds do not influence strongly the Vanadium Knight shift in the high temperature range. Over the entire range from 300 K up to 1300 K the magnitude of $K_{^{51}V}$ in V_3Ga is about 6% higher than the corresponding one in V_3Si.

A qualitative interpretation of the temperature dependence of $K_{^{51}V}$ and $K_{^{71}Ga}$ in V_3Ga may be given in the frame of a model which has been used earlier to explain the results of Knight shift measurements of transition metal systems [4, 5]. In this model, the temperature dependence of the Knight shift K is assumed to be associated only with the d-spin contribution K_d. The measured Knight shift K is separated as follows:

$$K(T) = K_s + K_d(T) + K_{orb}\,, \tag{1}$$

where K_s and K_{orb} are the s-electron and orbital contributions to the total Knight shift, respectively. The diamagnetic term and the higher order terms in (1) are negligibly small [6–8]. Additionally it is assumed that K_s and K_{orb} are positive, whereas K_d is negative [3, 6]. The negative sign of K_d results from estimates of the hyperfine fields associated with the core polarization due to half-filled d-shells. The estimates are based on experimental data and on exchange polarization calculations in the frame of the Hartree-Fock theory [9].

Now for the vanadium Knight shift $K_{^{51}V}$ in V_3Ga the positive contributions K_s and K_{orb} are dominant. With increasing temperature the absolute value of the negative K_d contribution decreases, and consequently the total value of $K_{^{51}V}$ in (1) increases. This explains our experimental results plotted in Figure 1. As experimentally found, the Gallium Knight shift $K_{^{71}Ga}$ is negative over the entire temperature range and shows a decreasing absolute value with increasing temperature (Figure 2). This behavior can be inter-

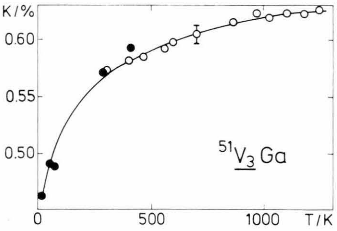

Fig. 1. The ^{51}V Knight shift $K_{^{51}V}$ in the V_3Ga compound as a function of temperature. (○ present work, ● reference [1]).

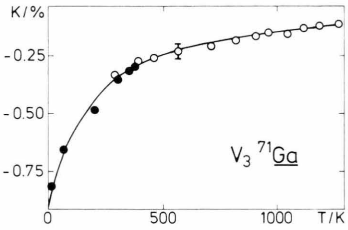

Fig. 2. The ^{71}Ga Knight shift $K_{^{71}Ga}$ in the V_3Ga compound as a function of temperature. (○ present work, ● reference [1]).

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preted using the above model with the additional assumption that the dominant hyperfine field at the position of the Ga nucleus is due to the K_d contribution. The mechanisms which cause the negative hyperfine field at the Ga nucleus are related with a strong mixture of the Ga 4p band with the V 3d band at the Fermi energy.

For a quantitative analysis of the electronic structure of the V_3X compounds in the high temperature range we need further experimental results. The experimental procedure of sample preparation and the high temperature spectrometer used for the measurements have been described elsewhere [3, 10].

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