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Thermodynamic, transport and magnetic properties of α'-NaV_2O_5

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Up to now α'-NaV_2O_5 has been described as a $S = \frac{1}{2}$ one-dimensional antiferromagnet which undergoes a spin–Peierls (SP) transition at $T_{SP} = 34$ K [1]. However, recent measurements raised some doubts if this description in terms of charge ordered chains is correct [2]. In this article we report on specific heat, electrical resistivity and ESR experiments on α'-NaV_2O_5. The ESR and resistivity experiments were performed on a high-quality needle-shaped single crystal. The heat capacity experiments were performed on polycrystalline material. The sample preparation and experimental details are described elsewhere [3,4]. Fig. 1 shows the ESR intensity which is a direct measure of the spin susceptibility. The overall behaviour of the susceptibility is in good agreement with DC results [1]: for $T > 250$ K it is well described by the Bonner–Fisher (BF) model (solid line) assuming a single-exchange constant $J = 578$ K. According to the model predictions $\chi_{\max} \approx 0.147 g^2 \mu_B^2 / J \approx 4 \times 10^{-4}$ emu/mol is expected close to the experimentally observed value $\chi_{\max} \approx 4.2 \times 10^{-4}$ emu/mol. While we find a good agreement at high temperatures, the experimental data decrease significantly faster than predicted towards lower temperatures. A possible explanation could be the increasing importance of three-dimensional exchange interactions. The inset of Fig. 1 shows the low-temperature data which are well described assuming $T_{SP} = 34$ K and an exponential decrease with a gap value of $\Delta = 100$ K (solid line in the inset of Fig. 1).

The heat capacity was measured for temperatures $3\text{ K} < T < 70$ K. In the analysis of our specific heat results we tried two parameterizations to describe the data for $T > T_{SP}$. In scenario A we fixed the linear term to the value calculated from the exchange interaction, namely $\gamma = 1.21 \times 10^{-3}$ R/K and fitted the phonon contribution. The best fit was obtained using a Debye temperature $\Theta_D = 281$ K and a number of degrees of freedom $N = 15$, but the specific heat anomaly at T_{SP}, $\Delta C/\gamma T_{SP} \approx 20$, was far off the mean-field (MF) value. In scenario B we fixed the magnetic specific heat to the MF prediction $\Delta C/\gamma T_{SP} \approx 1.4$, to reproduce the MF jump in the specific heat. From the fit in scenario B we deduced $\gamma = 19 \times 10^{-3}$ R/K, $\Theta_D = 302$ K and $N = 14$. A calculation of the exponential decrease of the specific heat with

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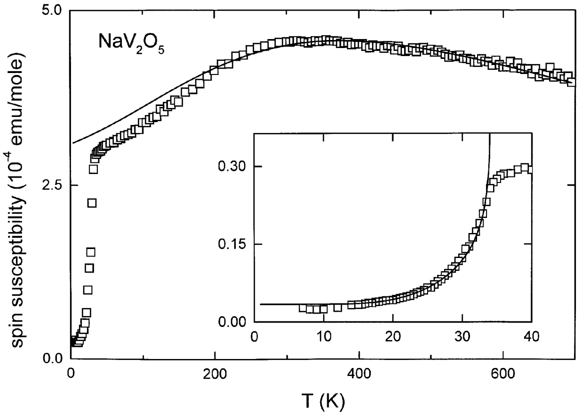

Fig. 1. ESR intensity in α'-NaV$_2$O$_5$ compared to the Bonner–Fisher model (solid line). The absolute value was determined by comparison to SQUID-measurements at 300 K. Inset: Spin susceptibility at low temperatures around T_{SP}. The solid line is a mean-field calculation with a gap of 100 K.

a constant gap value of 100 K and $T_{\mathrm{SP}} = 34$ K reveals a strong excess specific heat for temperatures below 20 K. The calculations of scenario B are roughly compatible with the experiment, but now the linear term is a factor of 15 too large compared to the predictions of the Bonner–Fisher model for a uniform AFM spin chain. Therefore, it has to be stated that the release of entropy at the phase transition is far too high for a spin–Peierls system with an exchange constant $J = 578$ K. The resistivity reveals a clear semiconducting behaviour and increases from 10^3 Ω at 600 K to almost 10^{13} Ω at low temperatures. Using high excitation voltages allowed to extend the measurements down to 20 K. A clear but smeared out anomaly at T_{SP} was detected and a strong decrease of the resistance by almost 40% within a range of 5 K above T_{SP} is observed. However, $R(T)$ increases again below T_{SP} for decreasing temperature, thus indicating semiconducting behaviour.

In conclusion, we presented ESR, specific heat and electrical resistivity results which can hardly be described within the framework of a spin–Peierls transition. The spin susceptibility at high temperatures can be well described by a Bonner–Fisher model, but shows significant deviations below 250 K. The heat capacity data are not compatible with a specific heat anomaly as predicted by a mean-field theory. The electrical resistivity shows semiconducting behaviour and a clear anomaly at T_{SP}.

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