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HIGH-FIELD MAGNETIZATION IN THE MOTT-HUBBARD SYSTEM (Y,Ca)VO₃

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We measured the magnetization of Y_{1-x}Ca_xVO₃ compounds with 0 ≤ x ≤ 0.6 in pulsed magnetic fields up to 56 T. YVO₃ exhibits a slightly S-shaped magnetization curve with an inflection point at B_c = 42 T. The critical field B_c was found to decrease with increasing calcium content, and no sign of an S-shape is seen for the compound with x = 0.6, which is at the boundary of the metal-to-insulator transition. Our data provide further evidence that the metal-to-insulator transition in this system coincides with the transition from a paramagnetic to a magnetic ground state.

1 Introduction

Strong on-site Coulomb repulsion between 3d electrons can cause an integer-filled (3d^N) system to be insulating. This leads to a possible formation of a Mott insulator, where the charge gap is determined by the Hubbard splitting (U) of the d band [1]. YVO₃ is such a Mott insulator and it exhibits two magnetic transitions at about 120 and 85 K [2]. The interactions in the phase AF1 (85 K < T < 120 K) are predominantly antiferromagnetic, while an additional small but significant ferromagnetic component was established for the low-temperature magnetic phase AF2 (T < 85 K). The Mott-Hubbard compound CaVO₃, on the other hand, is non-magnetic and it exhibits metallic conductivity at low temperatures [3]. Substitution of calcium onto the yttrium sites in YVO₃ causes an insulator-to-metal transition at about 60% of calcium content [4].

2 Sample Preparation and Characterization

We prepared 11 different $Y_{1-x}Ca_xVO_3$ compounds with increasing Ca content with a step size of $x = 0.1$. All samples were prepared by mixing stoichiometric amounts of high-purity starting material of Y_2O_3 , V_2O_3 , CaO and VO . After subsequent annealing under Ar and H atmosphere at 1000-1300°C, the polycrystals were grown using the floating-zone method. The quality and homogeneity of the samples was checked by X-ray diffraction, and the oxygen content was determined by thermal-gravity analysis. In all cases, we found single-phase samples with the desired oxygen content close to 3 (within 2%).

Next, we measured the magnetic susceptibility and electrical resistivity of all $Y_{1-x}Ca_xVO_3$ samples. Two magnetic transitions were found in YVO_3 and $Y_{0.9}Ca_{0.1}VO_3$, while only one magnetic transition could be identified for compounds with $0.2 \leq x \leq 0.6$. No magnetic ordering was detected for compounds with $x > 0.6$. The transport measurements revealed high room-temperature resistivity values and insulating behaviour for $x \leq 0.6$, while samples with higher Ca content show a more metallic behaviour. The results are summarised in Fig. 1.

Figure 1. Concentration dependence of the ordering temperatures (circles, left axis) and room-temperature resistivity values (triangles, right axis) of $Y_{1-x}Ca_xVO_3$ compounds. Note, that a metal-to-insulator transition occurs around $x = 0.65$, which is close to a paramagnetic-to-(antiferro)magnetic transition. Lines are guides to the eye.

3 High-Field Magnetization: Procedure and Results

The magnetically-ordered $Y_{1-x}Ca_xVO_3$ compounds with $0 \leq x \leq 0.6$ were ground to fine powders, which could be considered to consist of single-crystalline particles. The magnetization experiments were performed at 4.2 K on powders with particles free to be rotated by the applied field using a pulsed magnet at the High-

Field Facility in Osaka, Japan. Data were collected on field-oriented powders during the field-down sweep. This way, the magnetic response is believed to represent the easy-axis response of the material.

Fig. 2a shows the change in the magnetic response of YVO_3 and $\text{Y}_{0.9}\text{Ca}_{0.1}\text{VO}_3$. Compared to YVO_3 , $\text{Y}_{0.9}\text{Ca}_{0.1}\text{VO}_3$ exhibits a substantially large high-field susceptibility. Since only the change in magnetization is recorded, these experiments do not provide any measure of a possible spontaneous moment that is present in the AF2 phase, which is believed to be the ground state of these two compounds. Both compounds exhibit slightly S-shaped magnetization curves with inflection points B_c that we determined from the maxima in the derivative dM/dH (see inset of Fig. 2a). In Fig. 2b, the magnetic response of the other $\text{Y}_{1-x}\text{Ca}_x\text{VO}_3$ is shown. For these compounds (with an AF1 ground state), the overall magnetization decreases with increasing Ca content. Similarly to the former two compounds, we find an S-shaped magnetization curve for all samples except for $\text{Y}_{0.4}\text{Ca}_{0.6}\text{VO}_3$. For the other compounds, the inflection points B_c are found decrease approximately linear with increasing Ca content (see Fig. 3), and an extrapolation indicates that $B_c \rightarrow 0$ T for $\text{Y}_{0.4}\text{Ca}_{0.6}\text{VO}_3$.

Figure 2. Magnetic response of $\text{Y}_{1-x}\text{Ca}_x\text{VO}_3$ compounds at 4.2 K with Ca concentration x of a.) 0.0 and 0.1 and b.) 0.2, 0.3, 0.4, 0.5 and 0.6. In the inset, the derivative of the magnetization as a function of applied field is shown for the first two compounds. The arrows indicate the positions of the critical fields B_c .

4 Conclusion

We measured the magnetic response of magnetically-ordered $\text{Y}_{1-x}\text{Ca}_x\text{VO}_3$ compounds in magnetic fields up to 56 T. S-shaped magnetization curves provide evidence of a critical field B_c , at which antiferromagnetic interactions start to break up. However, these compounds show no (or little) tendency toward saturation even

Figure 3. Concentration dependence of the critical field B_c in magnetically-ordered $Y_{1-x}Ca_xVO_3$ compounds.

at the highest field applied. Increasing the Ca content decreases the critical field B_c , and no S-shape is found for $Y_{0.4}Ca_{0.6}VO_3$ which is at the boundary of the insulator-to-metal transition. Thus, we may argue that strong antiferromagnetic interactions are responsible for the insulator-to-metal transition in the $Y_{1-x}Ca_xVO_3$ system.

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