Complex magnetism in Fe_2VSi

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Abstract

Magnetic susceptibility and ^{51}V NMR measurements are reported for two samples of the Heusler alloy Fe_2VSi. Both samples have been quenched, one after annealing at 1073 K (sample 1) and the other at 1123 K (sample 2). The susceptibilities of both samples have been found to depend strongly on the applied static magnetic field. A new magnetic transition is found at 300 K for sample 2. NMR line widths of ^{51}V become appreciably broader at 80 K for sample 1 and at 150 K for sample 2. These temperatures do not correspond to the magnetic and crystallographic transition temperatures determined by diffraction experiments. The NMR widths are governed by the combined effects of the hyperfine fields from ferromagnetic iron clusters in the crystals and the intrinsic antiferromagnetic spin structures.

Key words: Fe_2VSi; magnetism; NMR

1. Introduction

Heusler-type compounds have received renewed interest owing to their ferromagnetic shape memory, half-metallic ferromagnetic or half-metallic antiferromagnetic properties. One of them, Fe_2VSi is reported to order antiferromagnetically below 123 K, at which temperature the material undergoes a structural phase transition from a high temperature cubic phase to a low temperature tetragonal modification [1], [2]. From Mössbauer spectra [1] the magnetic moment of the Fe atoms was estimated to be 0.22 μ_B. The effective moment determined from high temperature static susceptibility was reported to be 1.87 μ_B which gives a moment (gS) of 1.12 μ_B per iron atom [1]. A band structure calculation within the LMTO-CPA approximation predicts 0.37 μ_B per iron atom [3]. In view of these somewhat conflicting results, neutron diffraction experiments have recently been performed on two samples of Fe_2VSi. Both samples were quenched, one from 1075K (sample 1) and the other after annealing at 1123K (sample 2) [4]. The samples transform to a tetragonal structure at 112 and 103 K, respectively. At the first order phase transition long-range magnetic order is also established. Sample 1 has a simple antiferromagnetic structure with a moment of 0.9 μ_B per Fe atom at low temperature, whilst sample 2 undergoes a further transformation to an incommensurate magnetic structure below 67K with a moment of 0.58 μ_B per Fe atom [4]. The effective paramagnetic moments yield a moment per Fe atom (gS) of 0.9 μ_B and 1.5 μ_B for sample 1 and 2, respectively [4]. Neutron scattering experiments indicate that due to the heat treatment both samples differ in the degree of atomic order [4]. The purpose of the present study is to carry out NMR experiments of ^{51}V on the same samples of Fe_2VSi used in the neutron diffraction experiments.

2. Results and Discussion

The method of sample preparation is described elsewhere [4]. A SQUID magnetometer (Quantum Design

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MPS-2) was used for the susceptibility measurements. A home-built, phase-coherent pulsed NMR spectrometer was used for the ^{51}V NMR. The temperature dependence of the static magnetic susceptibility in an applied field of 15 kOe is shown in Fig.1 for the two samples. Both samples show a small peak at 67K, but no anomaly at the Neel temperature of 112 K. An anomaly is observed at 300 K for sample 2. Susceptibility measurements at low fields show more complicated behavior: Sample 1 shows two weak anomalies at 65 and 90 K in a field of 100 Oe, while sample 2 shows a large rectangular peak around 300 K together with a broad peak at 23 K. These data suggest that the spin structure in Fe_2VSi depends on the applied field and is more complicated than previously reported.

For both samples the width of the field-swept NMR spectrum of ^{51}V is quite sharp at high temperature and exhibits satellite signals for both samples. The NMR shift of the main peak is nearly zero for both samples. The temperature dependence of the half-width of the field-swept NMR spectra for both samples at an operating frequency of 17 MHz are shown in Fig.2. For sample 1, the width increases gradually with decreasing temperature becoming more rapid at temperature below about 80 K. The width for sample 2 remains sharp with decreasing temperature down to 150 K, but increases below 150 K with a more pronounced increase below 30 K.

For both samples the temperature dependence of the width does not scale with the susceptibility of Fig.1 and again there is no anomaly at the Neel temperature for both samples. These data seem to indicate that the NMR widths are governed by the combined effects of hyperfine fields from ferromagnetic iron clusters in the crystals as well as the intrinsic antiferromagnetic spin structures. These features are consistent with a detailed zero-field NMR study in a ferromagnetic, ternary $Fe_{3-x}V_xSi$ system ($0 < x < 0.75$) in which the NMR spectra were interpreted using local environmental configurations [5].

In summary, the present magnetization and NMR data support recent neutron diffraction experiments in which the antiferromagnetism in Fe_2VSi is found to strongly depend on the degree of atomic disorder.

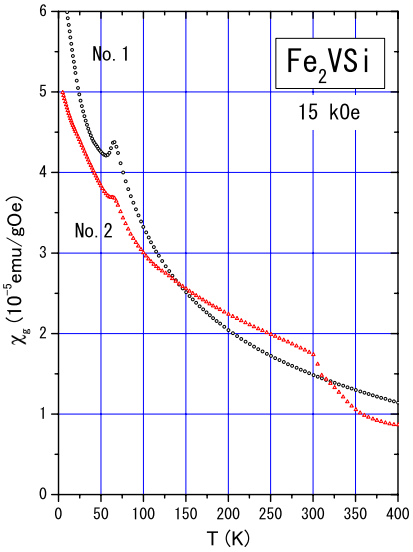

Fig. 1. Temperature dependence of the static magnetic susceptibility in an applied field of 15 kOe.

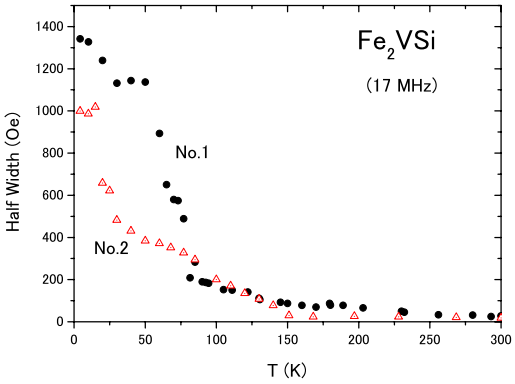

Fig. 2. Temperature dependence of the half-width of the field-swept NMR spectra at 17 MHz.

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