Low temperature specific heat enhancement in Fe_2VGa

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Abstract

Low-temperature specific heat measurements on the Heusler-type compounds Fe_2VGa have been performed. We observed the sample-dependent upturn in C/T at low temperature which is attributed to the effect of magnetic impurities and/or clusters. After subtracting this extrinsic effect, the resulting γ still indicated heavy fermion behavior with an effective mass of about 20 - 30 times larger than the value extracted from NMR results. Possible mechanisms for such an enhancement will be discussed.

Key words: Heusler compounds; specific heat; heavy fermion; spin fluctuations

The Heusler-type compound Fe_2VGa has been characterized as a semimetal, according to several theoretical calculations[1,2] and a recent nuclear magnetic resonance (NMR) study [3]. However, the electronic specific heat coefficient (γ evaluated as the low-temperature limit for C/T) was found to approach 20 mJ/mol K^2, relatively large given the low carrier density of this alloy [4]. Similar specific heat enhancements were also observed on other Heusler compounds Fe_2VAl and Fe_2TiSn [5,6]. Both materials have been proposed to be candidates for $3d$ heavy fermions.

A magnetic field-dependent specific heat investigation, however, indicated that the large low-T specific heat of Fe_2VAl was attributed to a Schottky-type anomaly, leading to false indications of heavy fermion behavior. Therefore, it is likely that a considerable portion of the observed γ in Fe_2VGa results from extrinsic effects, a finding reminiscent of the behavior of Fe_2VAl [7]. In this case, the corresponding low-T upturn in C/T is manifested by magnetic defects which would be sample-dependent. Thus, an investigation of different samples of Fe_2VGa in the specific heat can help identify these effects.

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Two samples studied here were prepared by an arc-melting technique. Annealing procedures for both samples were almost identical: homogenized at 600 °C for two days, and then further annealed at 400 °C for more than 12 h followed by furnace cooling. An x-ray analysis showed the expected $L2_1$ structure with no signs of a second phase for both substances.

Specific heat was measured in the temperature range 0.6–26 K with a ^{3}He relaxation calorimeter using the heat-pulse technique. The C/T vs T^2 plot below 26 K is demonstrated in Fig. 1. Low-T upturns in C/T were observed in our samples. As one can see, the feature of low-T upturn is sample-dependent. This provides convincing evidence that effects leading to such an upturn are not intrinsic properties of the Fe_2VGa system. The observed low-T upturn in C/T is possibly due to magnetic defects, similar to those found in Fe_2VAl [7].

With increasing temperature, the data taken from different samples converge together. The high-temperature specific heat is thus believed to be intrinsic and is a combination of electron and lattice excitations. We have fit the data between 15 K and 26 K to $C/T = \gamma T + \beta T^3$. The first term represents the standard electronic contribution while the remaining term is due to phonon contributions. (The next term in the anharmonic expansion, T^5, we found not to be significant.) This fit, shown as a dotted line in Fig. 1, yielded $\gamma = 9.9$ mJ/mol K^2 and $\beta = 0.065$ mJ/mol K^4. The $T = 0$ Debye temperature can be obtained from $\Theta_D = (234\ \mathrm{R}/\beta)^{1/3}$, where R is the ideal gas constant, yielding $\Theta_D = 310$ K for Fe_2VGa.

While the low-T upturn in C/T could be associated with Schottky anomalies, the extracted γ is considerably large as viewed from its semimetallic characteristics. The determined value of $\gamma = 9.9$ mJ/mol K^2 corresponds to a Fermi-level density of states $g(\varepsilon_f) \sim 4$ states/eV atom. On the other hand, NMR T_1 measurements yielded a smaller result: $g(\varepsilon_f) = 0.085$ states/eV atom was reported [3], extrapolated from V-site local density of states. This makes an estimate of total $g(\varepsilon_f)$ ~ 0.17 states/eV atom, taking even contributions from V-dominated electron pockets and Fe-dominated hole pockets at the Fermi level. The NMR T_1 is weakly enhanced by electron-electron interactions in normal metals, in contrast to the susceptibility, so in that case the T_1 can be considered to measure the band density of states. Compared to these results, γ is enhanced by a factor in the range of 20-30. Enhancement of γ can be due to electron-phonon (λ_{ep}) and electron-electron (λ_{ee}) effects. It is unlikely that the λ_{ep} term is significantly large, so we attributed the electronic mass enhancement to the λ_{ee} term.

For the specific heat of Fe_2VGa to be consistent with its semimetallic characteristics, the large value of λ_{ee} must be explained. Although the heavy fermion effect can not be ruled out for the present case of Fe_2VGa, a more realistic interpretation is the effect of spin fluctuations. Spin fluctuation behavior can provide a large λ_{ee}, but with a nearly divergent Stoner enhancement factor, since λ_{ee} depends on its logarithm [8]. This would be appropriate, since Fe_2VGa is nearly ferromagnetic, with T_c going to zero in $Fe_{2+x}V_{1-x}Ga$ at the Fe_2VGa composition [9]. It is therefore possible to explain the behavior of Fe_2VGa as a Stoner enhanced paramagnet. Measurements of the Pauli susceptibility would be useful in verifying the spin fluctuation mechanism, although this may be difficult due to the small $g(\varepsilon_f)$ and presence of magnetic defects.

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Fig. 1. Plot of C/T vs T^2 below 26 K for two Fe_2VGa samples. The dotted curve is the fitted function described in the text.

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