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Thermal expansion study of $Fe_{1-x}Co_xSi$

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Abstract

We present measurements of the linear expansion coefficient, α, on $Fe_{1-x}Co_xSi$ from 40 to 300 K and for $x = 0$, 0.02, 0.05, and 1. For the semiconducting samples ($x = 0$, 0.02, and 0.05) the results below 200 K are consistent with the presence of a small gap in the quasiparticle excitation spectrum; above 200 K there is an anomalous contribution to the thermal expansion that lacks a detailed explanation, but which is probably associated with the high density of conduction electrons found in FeSi above 200 K.

FeSi is a narrow-gap semiconductor that strongly resembles a Kondo insulator in many of its physical properties. Aeppli and Fisk [1] suggested that this resemblance is no accident but is in fact a manifestation of similar underlying physics. If this view is confirmed, it opens up the exciting possibility of studying heavy fermion phenomena at high temperatures.

Thermal expansion is a good probe of strongly correlated systems because the electronic Gruneisen parameter, which links the electronic part of the specific heat to the electronic part of the thermal expansion, is generally large in such systems. Recently, the thermal expansion of the Kondo insulator $Ce_3Bi_4Pt_3$ was shown to be amenable to a Gruneisen analysis [2]. Here we will not pursue such an approach but will instead concentrate on how the effects of a narrow energy gap are expected to appear in the thermal expansion.

$Fe_{1-x}Co_xSi$ crystals were prepared by arc melting high purity iron (99.98%) and silicon (99.9995%) into rod-shaped ingots which were subsequently zone refined. The crystals used in the thermal expansion measurements were characterized by X-ray diffraction, resistivity, and magnetic susceptibility. Good agreement with previous work [3] was obtained.

The thermal expansion measurements were performed using a capacitance dilatometer similar to that described by Brandli and Griessen [4] but with several modifications and improvements [5]. The change in the sample's length, ΔL, was measured at 5 K intervals and the linear expansion coefficient, $\alpha = (1/L)\mathrm{d}L/\mathrm{d}T$, was determined by differentiating a cubic spline interpolation.

Figure 1 plots $\alpha(T)$ versus T obtained on four samples with compositions as indicated. For reasons discussed at length in Jaccarino et al. [6], the lattice contribution to the specific heat and thermal expansion is expected to be similar in FeSi and (isostructural) CoSi. Therefore, the difference in the expansion coefficients can be ascribed to the electrons.

The specific heat of a narrow-gap semiconductor is expected to show a Schottky contribution [7] of the form

$$C_s = Nk_B\left(\frac{\Delta}{k_BT}\right)^2 \frac{g_0}{g_1}\frac{\exp(\Delta/k_BT)}{(1+(g_0/g_1)\exp(\Delta/k_BT))^2}, \quad (1)$$

where N is the number of particles, and g_0 and g_1 are the respective degeneracies of levels separated by a gap Δ.

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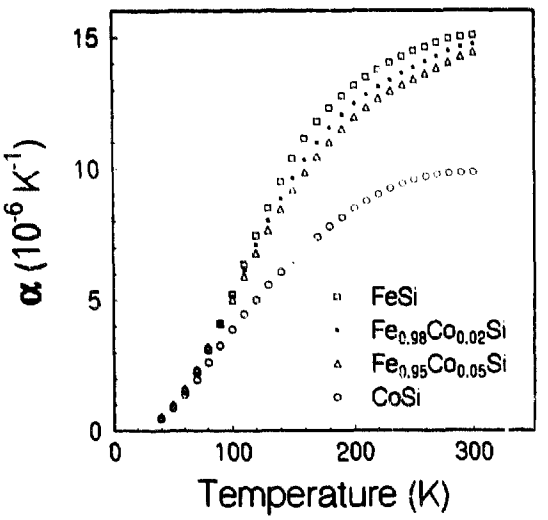

Fig. 1. Linear expansion coefficient, α, versus temperature for $Fe_{1-x}Co_xSi$ with $x = 0$, 0.02, 0.05, and 1.

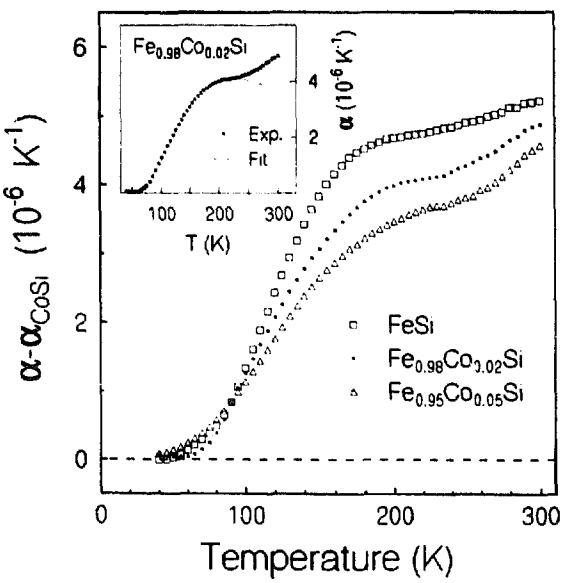

Fig. 2. Difference in linear expansion coefficients, $\alpha - \alpha_{CoSi}$, between three $Fe_{1-x}Co_xSi$ samples and CoSi. This difference represents the electronic contribution to the thermal expansion and is primarily the result of a small gap in the quasiparticle excitation spectrum (see text). Inset: $\alpha - \alpha_{CoSi}$ versus temperature for $Fe_{0.98}Co_{0.02}Si$ (dotted line) and fit using Eq. (1) (dashed line).

This Schottky term will be reflected in the thermal expansion according to the relation $\gamma = \beta V/\chi_s C_p$, where β is the volume coefficient of thermal expansion ($\beta = 3\alpha$ for cubic materials), γ is the Gruneisen parameter, χ_s is the adiabatic compressibility, and C_p is the heat capacity at constant pressure. If the Gruneisen parameter remains roughly constant, we expect a Schottky-type peak in the thermal expansion coefficient with $\Delta/T_{peak} \cong 2.4$ for $g_1 = g_0$ [7]. This effect is beautifully confirmed in the thermal expansion of $Ce_3Bi_4Pt_3$ [2].

Figure 2 plots $\alpha - \alpha_{CoSi}$, which represents the electronic contribution to the thermal expansion. It is clear from the figure that, although there is a large Schottky component to the expansion, there is also an anomalous piece that develops rapidly above 200 K. This piece is probably due to the expansion associated with free carriers, but whether a narrow-gap model can quantitatively explain it requires further study. Fits to the Schottky region (Δ assumed independent of temperature, $g_0 = g_1$) yield $\Delta = 540$ K for all three compositions. This value agrees reasonably well with $\Delta = 600$–700 K obtained from Arrhenius plots of the resistivity of FeSi. The fits also indicate that the main effect of adding cobalt is simply to reduce N, the number of carriers contributing to the Schottky component.

In conclusion, the thermal expansion of FeSi below 200 K is that of a good narrow-gap semiconductor. Above 200 K there is an anomalous contribution to the thermal expansion which is as yet unexplained. It remains to be seen whether a careful application of degenerate semiconductor statistics can explain the many anomalies observed near $T \cong 200$ K in FeSi, or whether more exotic theories are required.

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