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Elastic properties of FeSi

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Abstract

We present measurements of the complete elastic constants of single-crystal FeSi using resonant ultrasound spectroscopy (RUS). FeSi is a narrow-gap (0.05 eV) semiconductor whose physical properties are similar to a class of compounds known as hybridization gap semiconductors or Kondo insulators. The narrow gap is reflected in the temperature dependence of the elastic moduli.

FeSi is a cubic, transition-metal, narrow-gap (0.05 eV) semiconductor which has been studied for over 30 years. Many of its physical properties show activated behavior, and its magnetic susceptibility exhibits a maximum near 500 K [1]. Recently, FeSi has attracted attention in the context of hybridization gap physics as a possible non-rare-earth Kondo insulator [2].

We present measurements of the elastic moduli of FeSi using Resonant Ultrasound Spectroscopy (RUS) [3]. RUS permits the determination of the complete elastic moduli of small single crystals, as well as measuring ultrasonic attenuation, as a function of temperature.

For most solids the elastic moduli vary with temperature according to the Varshni function [4]

$$c_{ij} = c_{ij}^0 - \frac{s}{e^{(\tau/T)} - 1}. \tag{1}$$

This form assumes an Einstein model for the excitations of the system and produces the familiar linear temperature dependence of the elastic moduli at high temperatures. Our measured moduli for FeSi are shown in Fig. 1. While the data are fit well by Eq. (1) below 200 K, at higher temperatures the data deviate significantly.

In order to fit the data better, we consider a deformation potential coupling which explicitly includes the contribution of conduction electrons to the elastic moduli through a rigid two-band model ($E(\boldsymbol{k}) = E^0(\boldsymbol{k}) + d_\Gamma(\boldsymbol{k})\varepsilon_\Gamma$, where $d_\Gamma(\boldsymbol{k})$ is defined as $\partial E(\boldsymbol{k})/\partial\varepsilon_\Gamma$, and ε_Γ is a symmetry strain) [5]. Such models have been successfully applied to the study of other dense Kondo systems such as CeNiSn [6] and SmB_6 [7]. Consider the free energy for conduction electrons with band index i and energy $E^i(\boldsymbol{k})$:

$$F_{el} = -k_B T \sum_{i,k} \ln\left[1 + \exp\left(\frac{\mu - E^i(\boldsymbol{k})}{k_B T}\right)\right], \tag{2}$$

where μ is the chemical potential. Explicitly calculating the symmetry elastic moduli, $c_\Gamma = \partial^2 F/\partial\varepsilon_\Gamma^2$, and assuming conservation of the total number of quasiparticles [5] yields

$$c_\Gamma = c_\Gamma^0 - \frac{1}{k_B T}\sum_k d_\Gamma^2(k) f_k(1 - f_k) + \frac{1}{k_B T}\frac{\left(\sum_k d_\Gamma(k) f_k(1 - f_k)\right)^2}{\sum_k f_k(1 - f_k)}. \tag{3}$$

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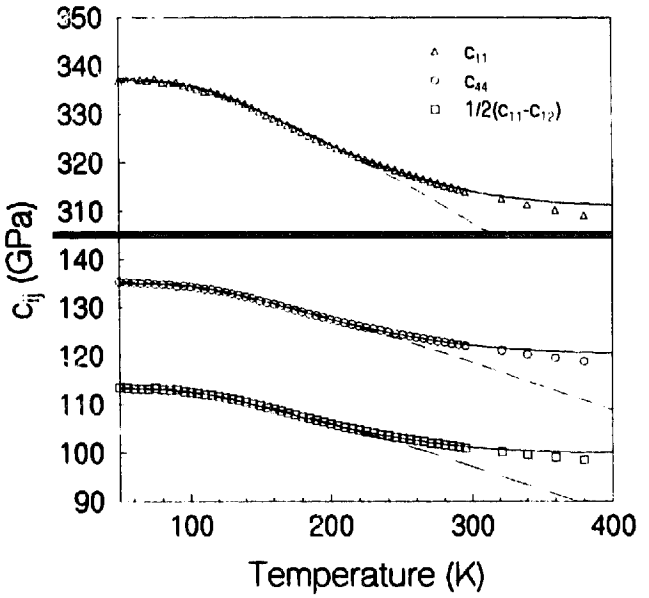

Fig. 1. Elastic moduli of FeSi as a function of temperature. The dashed curves are fits to the Varshni function (Eq. (1); for c_{11}, $s = 70.7$ GPa, $\tau = 365$ K; c_{44}, $s = 39.5$ GPa, $\tau = 366$ K; and for $1/2(c_{11} - c_{12})$, $s = 40.0$ GPa, $\tau = 374$ K). The solid curves are fits using a deformation potential coupling model. The parameters for these fits are given in Table 1.

where the band index is suppressed, f_k is the Fermi distribution function, and c_T^0 is the background elastic constant.

For simplicity, we assume a symmetric, rectangular density of states. Fitting this form to our data (see Fig. 1) yields the parameters in Table 1. While the fitted value of the gap is a little large and the bandwidths are unphysically small, the qualitative picture of a small gap between two narrow bands with large density of states does seem to reflect the fundamental physics of FeSi [1].

The small gap in FeSi can also be seen explicitly in ultrasonic attenuation. In Fig. 2 we show the temperature dependence of $1/Q$ (where Q for a resonance is defined as the center frequency divided by the FWHM) for one of the sample's resonance frequencies. A clear peak in the attenuation can be seen at 340 K. This peak is consistent with the activation energy, $\Delta/2$, as determined by transport.

Measurements of the elastic moduli reveal signatures of the narrow gap in FeSi. While the data are well-fit by a deformation potential coupling model, the fitted parameters are somewhat unphysical and point to the need for a more sophisticated model of the density of states or, perhaps, a temperature-dependent gap. Preliminary measurements of CoSi [8] also reveal that when the CoSi moduli are subtracted from the FeSi values to remove a lattice contribution, the temperature dependence of the resulting "electronic" contribution resembles the Schottky anomaly expected for a two-level system.

Table 1
Parameters used to fit the elastic moduli of FeSi. A symmetric, rectangular, rigid-band model with energy gap Δ, band width W, and density of states D is assumed

Modulus	Δ (K)	W (K)	$(d_T^{\downarrow} - d_T^{\uparrow})^2 D$ (GPa)
c_{11}	1295	12	13072
c_{44}	1296	17	4951
$\frac{1}{2}(c_{11} - c_{12})$	1250	7	10600

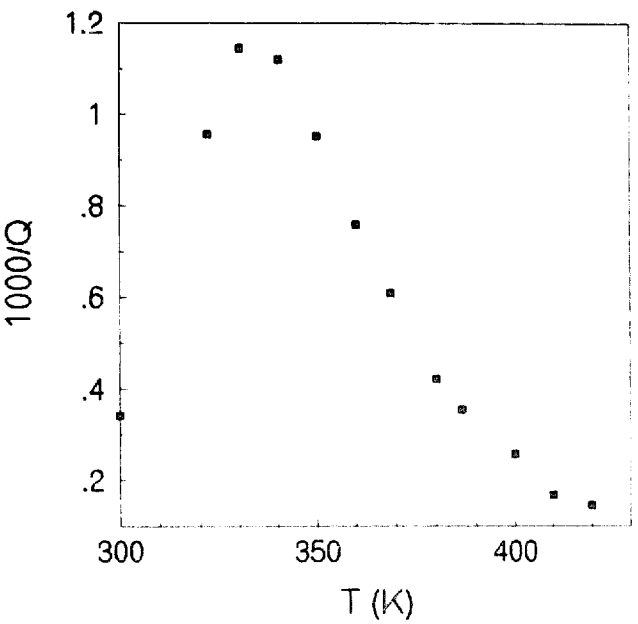

Fig. 2. $1/Q$, which is proportional to attenuation, is plotted for one of the measured resonance frequencies. The peak in attenuation occurs at the activation energy ($\Delta/2$).

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