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Transport and optical properties of FeSi

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Abstract

We have investigated the electrodynamic response of the cubic compound FeSi, including $\sigma_{\text{DC}}(T)$ and the optical reflectivity as a function of temperature over a very large frequency range, extending from the far infrared regime up to the ultraviolet spectral range. By lowering the temperature a gap excitation at about 800 cm^{-1} and several absorption peaks were found. Moreover, the spectral weight lost below the gap reappears just above it and is not distributed over an energy range of order eV, as suggested in previous work.

The cubic compound FeSi has raised appreciable interest in the past as a non-magnetic narrow-gap semiconductor [1], sharing several unusual properties with a class of rare-earth compounds known as hybridization-gap semiconductors or Kondo insulators [2]. Therefore, this compound appears suitable for investigating aspects of the electronic properties of a d-transition metal compound that might be related with features of correlation effects in f-electron materials.

A first optical investigation in the far- and mid-infrared frequency range suggests that FeSi is a dirty metal at high temperatures, while at low temperatures its optical conductivity resembles that of a semiconductor [3]. The striking but also puzzling feature is the redistribution of the missing spectral weight below the gap energy over a very broad frequency range, extending to several electron volts even beyond the measured photon energy range [3].

We were thus motivated to systematically study FeSi, by investigating a much broader energy spectral range from the far-infrared (FIR) and up to the ultraviolet. This study was performed on the same sample used for transport, magnetic and thermody-

namic investigations [4]. This is particularly relevant here since FeSi is not a line compound and there is evidence that even a small change in chemical composition may play an important role [4]. In this paper, the optical results are discussed together with the DC-transport properties.

The sample was grown in antimony flux and had the shape of a prism. Its resistivity $\rho(T)$, displayed in Fig. 1, was measured as a function of temperature between room temperature and 1.5 K, using a standard four-wire low frequency AC technique, with bare platinum or copper wires fixed to the sample by conducting silver paint [4]. As the temperature falls there is a monotonic rise in the resistivity by three and a half orders of magnitude at the lowest measured temperature of 1.5 K. On a linear scale there is a shoulder in the data at $T = 120 \text{ K}$, and a tendency to saturation below 10 K was observed (see inset of Fig. 1). In between, although the resistivity rises very steeply, it is nevertheless not possible, over any extended range of temperature, to describe the data with the usual activated behaviour, as would apply to a conventional semiconductor and contrary to what has been claimed in Ref. [3]. A fit to an expression appropriate to a variable-range hopping mechanism is, however, possible in this region [4]. The tendency to saturation

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Fig. 1. Temperature dependence of the resistivity $\rho(T)$. The inset displays the resistivity in the temperature range where the saturation of $\rho(T)$ takes place.

below 5 K suggests that the FeSi sample, far from being a semiconductor, is metallic in character in that temperature regime. This, following a steep rise in resistivity with decreasing temperature, suggests in turn that this arises through the formation of itinerant carriers from 'impurities'.

Reflectivity measurements, summarized in Fig. 2(a), were performed on a very broad frequency range, from the ultraviolet down to FIR (i.e. from 15 up to 10^5 cm^{-1}), and as a function of temperature, using four spectrometers with overlapping frequency ranges. The optical conductivity, shown in Fig. 2(b) was obtained from a Kramers–Kronig (KK) transformation applied to the measured optical reflectivity. Appropriate extrapolations were used above the highest frequency limit, while from the FIR down to zero frequency the reflectivity was extrapolated with the Hagen–Rubens law between 300 and 100 K, to a constant value for the spectra below 40 K. The relevant feature is the strong temperature dependence in the FIR, where the reflectivity changes from a metallic behaviour at temperatures larger than 100 K (i.e. it tends towards 100% for $\omega \rightarrow 0$) to a typically insulating one below 40 K. This may also be easily recognized in terms of the optical conductivity $\sigma_1(\omega)$, whose DC limit drops continuously (with the exception of the measurement at about 200 K) as the temperature decreases and below 40 K, is vanishingly small. The increase of $\sigma_1(\omega \rightarrow 0)$ at 200 K is related to the shallow minimum in $\rho(T)$ between 300 K and the above-mentioned shoulder at about 120–140 K. We also note the appearance of several sharp modes in the FIR frequency range upon decreasing the temperature. Our

Fig. 2. (a) Optical reflectivity of FeSi at 10, 120, 200 and 300 K, and (b) corresponding optical conductivity, obtained with Kramers–Kronig transformation (note the logarithmic energy axis). We note that the optical data below 40 K are identical to the reported spectrum at 10 K.

optical results are, at first sight, similar to those reported in Ref. [3].

As can be seen in Fig. 2(b), the Drude component in $\sigma_1(\omega)$ ascribed to the free charge carriers is progressively quenched down to 100 K and disappears below 40 K. Even though $\rho(T)$ still increases by orders of magnitude below 40 K, we are not able to detect any temperature dependence of $\sigma_1(\omega)$ in FIR, a frequency range characterized by an insulating-like optical conductivity. Nevertheless, our low frequency investigations at 10, 35 and 100 GHz, (to be fully reported elsewhere [5]), provide evidence for an enhancement of the conductivity, upon increasing both the frequency and the temperature.

Recent magnetic, thermodynamic and transport investigations can all be interpreted quantitatively by assuming Anderson-localized states associated with defects at the level of 10^{19} cm^{-3} [4]. However, the electrical conductivity, which was not activated, saturates below 6 K, thus suggesting a metallic state. The presence of itinerant charge carriers can be reconciled

with Anderson localization only by assuming that the Fermi level and the mobility edge coincide [4]. Consequently, only 4% of the Anderson-localized charge carriers ($\sim 4 \times 10^{17} \text{ cm}^{-3}$) are eventually delocalized [4]. This would correspond to a very small amount of spectral weight contributing very little to the optical conductivity. Our investigations in the millimeter, microwave and FIR frequency range seem to confirm this interpretation [5].

Apart from the sharp FIR modes (See Fig. 2(b)), there is another absorption at 770 cm^{-1} , which grows in intensity with decreasing temperature and which has been ascribed to excitations across a gap in the charge fluctuation spectrum [3]. Recent band structure calculations [6,7] suggest an indirect gap excitation around 0.1 eV. Our data indicate, furthermore, that a broad bump at approximately 450 cm^{-1} is overlapping this gap-like absorption. The origin of the FIR modes as well as of the latter absorption at 450 cm^{-1} is still controversial. Investigations are in progress, in order to single out whether phonons, as suggested in Ref. [3], or 'midgap' absorptions due to defect states or excitons are the appropriate interpretation for these excitations [5].

Finally, there are two important differences with respect to the results of Ref. [3] and in relation to the opening of the gap. First, assuming that the absorption at 770 cm^{-1} is reflecting the optical gap (although $\rho(T)$ does not show any activated behaviour), we note that this excitation persists up to 300 K. In Ref. [3], however, the filling and disappearing of the gap was monitored at temperatures lower than 200 K. Second, in our investigations which extend up to 12 eV, the spectral weight, removed at low frequencies upon decreasing the temperature down to 10 K, is relocated

around the absorption at 770 cm^{-1} . There is no need to integrate up to an anomalously large energy in order to recover the missing spectral weight, as suggested in Ref. [3]. In conclusion, we argue that the optical data do not make it necessary to invoke an energy scale much larger than the gap energy to understand the physics of FeSi.

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