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Investigation of the gapless state in $CuFeTe_2$

A A Vaipolin, S A Kijaev, L V Kradinova, A M Polubotko, V V Popov, V D Prochukhan, Yu V Rud and V E Skoriukin

A F Ioffe Physico-Technical Institute, Russia Academy of Sciences, Politekhnicheskaya 26, Sankt Petersburg, 194 021 Russia

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Abstract. The $CuFeTe_2$ ternary compound with a layered crystalline structure has been studied. The compound is paramagnetic in the temperature range 10–200 K. Investigation of the $\mu(T)$ temperature dependence demonstrates the ferron character of the carrier transport with the Mott diffusional mechanism. The obtained power dependences $n(T)$, $R(T)$ and $\sigma(T)$ allow us to conclude that $CuFeTe_2$ belongs to the gapless semiconductors. The temperature behaviour of $n(T)$, $R(T)$ and $\sigma(T)$ can be explained by examining features from the electron spectrum of $CuFeTe_2$ under conditions where the character of the carrier transport is close to the zone type and the general character of the spectrum is determined by the symmetry group and by the type of irreducible representation of the group.

In [1], the gapless state in the ternary compound $CuFeS_2$, which is a magnetic semiconductor of the I–VIII–VI_2 type, was reported. In this connection it is of great interest to investigate some isoelectronic analogues and their properties. In this work we present information revealing the gapless state in $CuFeTe_2$.

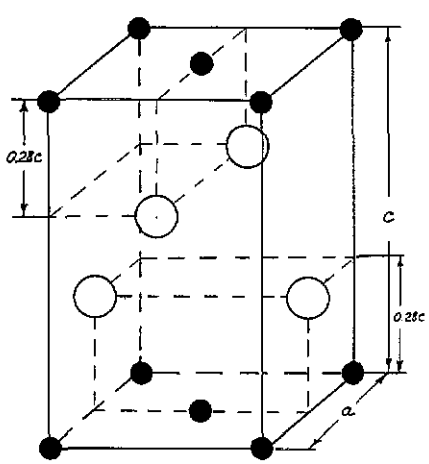

Figure 1. Crystal structure of $CuFeTe_2$ (a = 3.934 Å, c = 6.078 Å): ●, iron and copper atoms; ○, tellurium atoms.

The first communication about this substance appeared in [2]; however, until now its characteristics have not been studied. Our investigations enable us to state that

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it has the following properties. The crystalline lattice has been determined from x-ray studies (figure 1). The compound has a layered structure, where the copper and iron atoms are situated in the same layer and are positionally indistinguishable. Tellurium atoms are situated at the sides of the parallelepiped as shown in figure 1. Measurements of the magnetic susceptibility temperature dependence indicate that the specimens measured are typical paramagnets in the temperature range 10–200 K (figure 2). The ordered magnetic structure has not been revealed, although for some specimens it may certainly exist. Of great interest is the investigation of the temperature dependences of the following characteristics: specific conductivity $\sigma(T)$, Hall coefficient $R(T)$, carrier concentration $n(T)$ and electron mobility $\mu(T)$. In our experiments the $R(T)$- and $\sigma(T)$-values have been measured by the usual probe compensational method in constant weak electrical and magnetic fields in the temperature range 2–300 K. On the basis of these measurements the $n(T)$- and $\mu(T)$-values have been calculated using the well known phenomenological formulae

$$n = -1/eR \qquad \mu = -R\sigma. \tag{1}$$

Here it is taken into account that all the samples were n type. Typical dependences of $R(T)$, $\sigma(T)$, $n(T)$ and $\mu(T)$ are presented in figure 3. The analysis shows that in a wide temperature range these values have the unusual power dependences $R(T)$, $\sigma(T)$, $n(T)$, $\mu(T) \sim T^k$ where $k = -1.9$ for R, $k = 1.15$ for σ, $k = 1.9$ for n and $k = -0.75$ for μ. The absence of the exponential dependences of $n(T)$, $R(T)$ and $\sigma(T)$ demonstrates the absence of the forbidden gap in this compound. The power dependences of these values are characteristic of gapless semiconductors. Therefore we conclude that $CuFeTe_2$ belongs to a new class of compounds—gapless magnetic semiconductors.

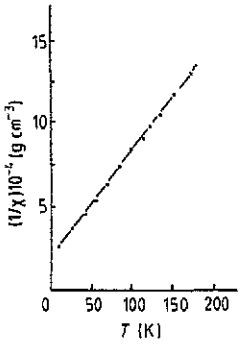

Figure 2. Temperature dependence of the reverse magnetic susceptibility.

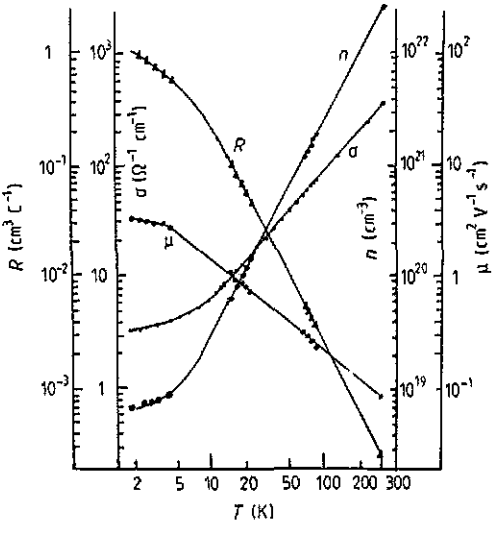

Figure 3. Temperature dependences of the specific conductivity σ, Hall coefficient R, electron concentration n and electron mobility μ.

The main peculiarity of the gapless state in $CuFeTe_2$ is that it is observed in the paramagnetic phase, where the applicability of the band theory to spectrum

description is questionable. We shall start our analysis with a consideration of the mobility temperature dependence. The power dependence obtained, $\mu \sim T^{-0.75}$, is close to that characteristic of a magnetic polaron (i.e. a ferron) of small radius. For the diffusional Mott mechanism of transfer [3],

$$\mu = ea_0^2/kT\tau\gamma^4 \sim 1/T \tag{2}$$

where a_0 is the radius of the region occupied by one magnetic atom, $\gamma = R_0/a_0$, R_0 is the ferron radius and τ is the spin relaxation constant. It is necessary to note that for another representative of this class of compounds, namely the gapless magnetic semiconductor $CuFeS_2$, the mobility temperature dependence $\mu(T) =$ constant [1] also indicates the ferron character of transport, but with large-radius ferrons [3]. Thus these two results are in good agreement with the nature of these compounds, which are magnets. It should be noted that the mobility temperature dependence for $CuFeTe_2$ differs slightly from (2). This may be caused both by calculation errors and the manifestation of deeper regularities.

The temperature dependences $n(T)$, $R(T)$ and $\sigma(T)$ for $CuFeTe_2$ have some features which distinguish this substance from the 'classical' gapless semiconductors of the first and second types for which $n(T) \sim T^3$ and $n(T) \sim T^{3/2}$, respectively. These dependences are $n(T) \sim T^{1.9}$, $R(T) \sim T^{-1.9}$ and the dependence $\sigma(T) \sim T^{1.15}$. Since the exact magnetic structure is not known it is impossible to perform a theoretical group analysis in order to prove the possibility of appearance of the gapless state. Moreover, it is impossible to determine an analytical form of the spectrum and therefore to calculate the temperature dependences $n(T)$, $R(T)$ and $\sigma(T)$. Another essential difficulty in doing this, even if the magnetic structure were known, is the ferron transport character of the carriers revealed. It is known that in order to obtain the analytical form of the spectrum $E(k)$ near the symmetrical point, one usually employs the $(k \cdot p)$ method, which uses as its basis the single-electron Bloch functions. However, the ferron transport character shows the essentially multielectron state of the carriers. The last obstacle may be avoided if we suppose that the general spectrum character of ferrons in the vicinity of the symmetrical point is determined by the symmetry group and by the type of irreducible representation, which describes their transformational properties. Using the similarity of $CuFeTe_2$ and $CuFeS_2$ which is expressed in the existence of the ferron states in both substances, one can check this assumption for the latter compound and satisfy oneself that it is in good agreement with the experimental results. Indeed, in accordance with [4] the gapless state in $CuFeS_2$ can be realized only at the P point of the Brillouin zone. Since the magnetic symmetry group of this compound is of a single-colour nature [4] all the results referring to the group D_{2d}^{12} which describes the symmetry properties of the $A^2B^4C_2^5$ compounds are applicable to $CuFeS_2$. In accordance with [5] the general dispersion law at the P point for the P_3 irreducible representation, obtained without using the ferron states, is the following:

$$E(k) = A(k_x^2 + k_y^2) + Bk_z^2 \pm \sqrt{C^2(k_x^2 - k_y^2)^2 + D^2k_x^2k_y^2 + Ek_z^2 + 2DEk_xk_yk_z} \tag{3}$$

where A, B, C, D and E are arbitrary constants. When k is small, the main term in (3) is Ek_z^2, which causes the spectrum character

$$E(k) \sim |k|. \tag{4}$$

This corresponds to a spectrum of the first type of gapless compounds and to the temperature dependence $n(T) \sim T^3$, which has been observed experimentally [1].

If we consider that the electron motion in $CuFeTe_2$ is of a zone character and use the above-mentioned hypothesis, then the temperature dependence obtained, i.e. $n(T) \sim T^{1.9}$, is close to $n(T) \sim T^2$ and may be caused by the fourth term in the square root of equation (2), when

$$E(k) \sim \sqrt{2DEk_xk_yk_z}. \tag{5}$$

Some deviation from the dependence $n(T) \sim T^2$ may be explained both by non-exact calculations and by the difference between the densities of the electron and hole states as well as by the fact that the specimens measured are n type. The last fact causes a slight temperature dependence of the Fermi level and therefore influences the temperature dependences $n(T)$, $R(T)$ and $\sigma(T)$.

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