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WEAK LOCALIZATION AND ELECTRON-ELECTRON INTERACTION IN THE LAYERED COMPOUND $CuFeTe_2$

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El estudio de las propiedades eléctricas del compuesto laminar CuFeTe2 indica que hay tres regímenes de conducción bien diferenciados dependientes de la temperatura. Por debajo de TSDW ~ 300 K se ha reportado la formación de un estado de Ondas de Densidad de Espín (SDW), en el marco de una transición metal no metal. Por debajo de 100 K (~ TSDW/3) el comportamiento de la resistencia eléctrica como una función de la temperatura y el campo magnético se atribuye a los electrones no condensados (cuasi partículas) en el estado SDW. A bajas temperaturas (1.8 - 20K), baja corriente (< 1 mA) y campo magnético (0 <H <6 Tesla), los efectos de localización débil e interacciones electrónicas aparecen. A temperaturas intermedias (20 < T < 100 K) se observa un comportamiento de conductividad hopping.

The study of the electrical properties of the layered compound CuFeTe2 shows that there are three well differentiated conduction regimes depending on the temperature. Below TSDW ~ 300 K the formation of a Spin Density Wave (SDW) state has been reported, in the frame of a metal to non metal transition. Below 100 K (~ TSDW/3) the behavior of the electrical resistance as a function of temperature and magnetic field is attributable to the still present not condensed electrons (quasi particles) in the SDW state. At low temperatures (1.8 - 20K), low current (< 1 mA) and magnetic field (0<H <6 Tesla), the effects of weak localization and electronic interactions in two dimensions appear. At intermediate temperatures (20 < T < 100 K) a hopping conductivity behavior is observed.

Palabras Clave. Localization effects 72.15.Rn, Hopping transport 72.20.Ee, Weak localization 73.20.Fz, Spin-density waves

INTRODUCTION

The systems of reduced dimensionality are the focus of attention of many studies in physics of the condensed matter. The electrons in these systems are confined to geometries that force them to strongly interact with each other, giving rise to a rich variety of behaviors and phase transitions. The free electron gas instability allows, at low temperatures, the appearance of states like superconductivity, or Charge Density Waves (CDW) or Spin Density Waves (SDW).

The SDW state, proposed by A. W. Overhausser in 1962[1], has been broadly studied in two prototypic families of materials, Cr and their alloys[2,3] and Bechgaard salts[4]. It has also been put in evidence that two dichalcogenide compounds, CuFeSe2 (quasi-1D system, TSDW = 71 K)[5] and $CuFeTe_2$ (quasi-2D system, T_{SDW} = 300 K)[5], present a SDW state. More recently thermodynamic and transport measurements in the layered compound Fe-oxypnictide, LaFeAsO, show a structural phase transition at Ts = 155K, which has been associated with the formation of a SDW state[6].

The SDW state in $CuFeTe_2$ is supported by previous magnetic susceptibility, electrical resistance and Mössbauer spectroscopy measurements[5,7,8] in a sample prepared by the Bridgman vertical growth technique. A magnetic transition is observed at 308 K, with a Pauli paramagnetism behavior above this temperature. The thermal evolution of the Mössbauer spectra between T_{SDW} and $T_{SDW}/3$ reflect the presence of the condensed state (a magnetically split wide distribution of hyperfine fields) and the normal state (a non magnetic contribution). A spectrum at low applied magnetic fields in the Pauli paramagnetic zone suggests the absence of localized magnetic moments on iron, confirming that the magnetic order observed is of itinerant origin. There is a metal to non metal transition, at T_{SDW} = 300 K, indicating the opening of a gap at the Fermi level. I-V measurements indicate a non linear electrical conductivity, which suggests the coexistence of two conduction channels, one associated with the normal electrons (ohmic conductivity) and the other one associated with the SDW state (non ohmic conductivity). This behavior is a consequence of the depinning and sliding of the SDW condensate[4].

The compound $CuFeTe_2$ crystallizes in a tetragonal structure with unit cell parameters of a = 3.934 Å and c=6.078 Å (space group P4/nmm, No. 129)[9], formed by conductive planes of Cu and Fe cations and planes of Te anions, perpendicular to the crystallographic c-axis. The layered structure is shown in figure 1. The anions are arranged in a tetragonal deformed fcc sublattice. Each Cu or Fe atom is surrounded by four Te atoms in tetrahedral coordination. Two adjacent planes of Te atoms are separated by Van der Waals gaps (figure 1) that allow the cleavage in directions perpendicular to

the c-axis. The overlap of 3d Cu and Fe orbitals in the cation planes is expected (minimum separation between cations is 2.81 Å). Such atomic metallic planes can be considered as conducting sheets of, say, 2 Å thickness.

The electrical transport properties of $CuFeTe_2$ were initially studied by Vaipolin et al.[10] by means of resistivity measurements as a function of temperature. Between 4.2 and 500 K, $\rho(T)$ decreases two orders of magnitude, wich a thermal variation given by $\rho(T) = cT^{-\beta}\exp(T_0/T)^x$ with x ~ 1 below 200 K.

F. N. Abdullaev et al.[11] have investigated the temperature dependences of the electrical resistivity of $CuFeTe_2$ semiconductor single crystals, parallel and perpendicular to the plane of the crystal layers, in the temperature range 5-300 K. The temperature dependence of the electrical resistivity presents two regions associated with different mechanisms of electrical conduction, thermally excited impurity charge carriers in the allowed energy band and hopping between localized states lying in a narrow energy band near the Fermi level.

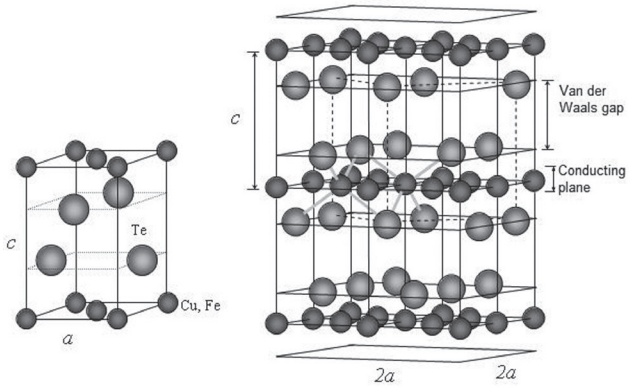

Figure 1. Crystalline structure of the $CuFeTe_2$ compound. Unit cell (left) and crystal (right).

In this work we present a detailed study of the compound $CuFeTe_2$ at low temperatures and high magnetic fields. In particular, we have measured the resistance as a function of the temperature along the conducting planes, as well as, the transverse magnetoresistance down to 1.8 K and up to 6 Tesla. The results suggest that the conduction in this system is determined by the effects of weak localization and electronic interactions in two dimensions.

2 EXPERIMENTAL TECHNIQUES

We have carried out a study of the electrical conduction on a new sample of $CuFeTe_2$ prepared by the standard melting and annealing technique of a stoichiometric mixture of each of the constituent elements. The layered sample obtained is of high quality, as it has been observed in the optical microscope, as well as, by x-ray diffraction. A monocrystalline sheet with a brilliant surface has been obtained by cleavage.

The measurements of the resistance as a function of temperature, between 1.8 and 290 K, and the magnetoresistance, in pulsed high magnetic fields up to 6 Tesla, were made in direct current (dc) using the standard four probe method. The sample selected for the study was approximately 0.35 mm thickness, cleaved (in the plane a-b) directly from the original ingot. The electric contacts were made using gold wires of 25 μm and silver paint. Due to the layered structure of the compound, the electric contacts were placed on the edge of the sample. This allows a better current distribution in many conducting planes. The sample was covered with vaseline to avoid the oxygen contamination, known to take place between the Var der Waals gaps, which cause their deterioration and the appearance of jumps in the resistance. The results are reproduced very well in the different thermal cycles and in high magnetic fields, indicating the stability of the sample.

RESULTS AND DISCUSION

Resistance vs temperature. Figure 2 shows the resistance as a function of temperature in log-log scale, between 1.8 and 290 K, for a current of 1 mA dc (ohmic regime). In the whole measurements interval a non metallic type behavior is appreciated, with a variation in R(T) of one order of magnitude. There exist three well differentiated conduction regimes: low, intermediate and high temperatures. Above 20 K a smooth change in the resistance takes place, say $R(T) = R_o T^{\beta}$, that can be attributed to hopping conductivity assisted by phonons. This dependence in temperature has been observed in $CuFeTe_2$ by Vaipolin et al.[9] and F. N. Abdullaev et al.[10]

The analysis of the $R(T)$ curve between 20 and 100 K by means of the logarithmic derivative technique $d(\ln R)/d(\ln T)$, allow us to determine the value of the parameter $\beta = -0.48 \pm 0.06$ (see insert of figure 2). On the other hand, the zero value of the slope in this figure indicates that thermal activation doesn't exist in this temperature range. Above 100 K the conduction in $CuFeTe_2$ is associated to the thermal evolution of the condensate fraction in the SDW regime[7], which decreases up to the non metal to metal transition (T_{SDW}), already observed in other samples of this system[7].

In the linear regime the condensate (the SDW) does'nt contribute to the conductivity. The SDW is pinned to the lattice by impurities, defects and imperfections, and only the non condensed electrons participate in the conduction. At low temperatures it is expected that only a small fraction of the conduction electrons is responsible for the behavior of the resistance in $CuFeTe_2$. The Mösbauer spectroscopy allowed us to observe simultaneously the fraction of condensed electrons (the magnetic SDW contribution to the spectra) and in the other hand the non condensed fraction (the non magnetic quadrupole doublet). The results indicate that almost 10% of the conduction electrons remain uncondensed at 4.2 K[7].

Magnetoresistance. The magnetoresistance was measured at 1.8, 4.2 and 20 K, in pulsed magnetic fields perpendicular to the sheets (conductive planes). A dc current of 5 mA was applied parallel to the sheets. The results indicate a negative magnetoresistance in the whole range of magnetic field.

The negative behavior of the magnetoresistance can be associated to the effects of weak localization in disordered 2D systems. In systems with CDW and SDW this behavior has

been observed, which is an indication of the disorder existing in those compounds.

To estimate the values of the sheet magnetoresistance, R_s, we look the sample as a parallelepipede of ≈ 2x1x0.35 mm^3. If the sample is assumed to be formed by 0.35mm/6.087x10-7mm = 5.76x10^5 sheets in parallel, with, say, d=2x10^{-7} mm metallic width (cations planes) per sheet and per unit cell (cell parameter c=6.087x10^{-7} mm), leading to a metallic effective thickness t_{ef}=5.76x 10^{5}x2x10^{-7} mm=1.152x10^{-1} mm, which gives a resistivity ρ=2.57x 10^{-2} Ω. cm and a sheet resistance Rs=ρ / d=1.29 MΩ at 1.8 K.

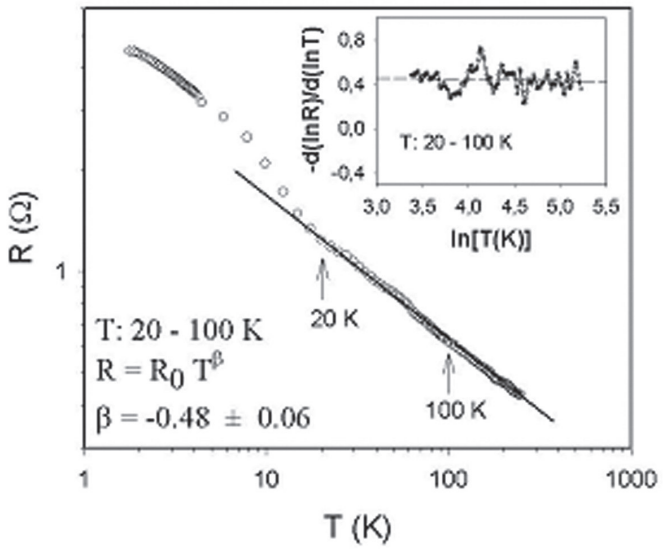

Figure 2. Resistance as a function of temperature in CuFeTe2.

According to the weak localization model in two dimensions[12,13], the magnetic field dependence of the magnetoresistance is given by

$$\frac{\Delta R_s}{R_s^2} = \alpha \frac{e^2}{2\pi^2 \hbar}\left[\frac{1}{2} f_2\left(\frac{H}{H_\varphi}\right) - \frac{3}{2} f_2\left(\frac{H}{H_2 + H_\varphi}\right)\right] \qquad (1)$$

where α is a parameter of the order of 1.
The characteristic fields H_φ and H_2 are defined as

$$H_\varphi = H_i + 2H_s \quad \text{y} \quad H_2 = \frac{4}{3}\left(H_{so} - H_s\right) \qquad (2)$$

and represent the different scattering mechanisms of the electrons, that is, inelastic (*i*), spin (*s*) and spin-orbit (*so*). The function f_2 is defined as

$$f_2(h) = \Psi\left(\frac{1}{2} + 1/h\right) + \ln h \qquad (3)$$

here Ψ is the digamma function.

The perturbation theory calculations up to first order show that the corrections to the conductivity, of the localization and electronic interactions, are additive. There is a correction term due to the electron-electron interactions which for 2D systems was calculated by P. A. Lee and T. W. Ramakrishnan[12] and is given by

$$\frac{\Delta R_s}{\Delta R_s^2} = \frac{F}{2}\frac{e^2}{2\pi^2\hbar} g_2\left(\frac{g\mu_B H}{k_B T}\right) \qquad (4)$$

where F is the Coulomb screening factor, that can be calculated only in the free electron model. Taking the electronic density ~ 5x10^{20}/cm^3 for $CuFeTe_2$, the value F=0.363 is obtained.

The function g_2 is given by the integral expression

$$g_2(h) = \int d\Omega \frac{d}{d\Omega}\left(\frac{\Omega}{e^{\Omega} - 1}\right) \ln\left|1 - \frac{h}{\Omega}\right| \qquad (5)$$

where $h = g\mu_B H / k_B T$.

With the values of R_s as a function of the magnetic field for each temperature, and the value of *F*, the contribution of the electronic interactions was calculated and it was subtracted from the experimental data. The curves of the resulting magnetoresistance (due to the effects of weak localization) are shown in figure 3 (circles). The solid lines correspond to the fitting by means of equation 1. In the weak localization regime, when increasing temperature and magnetic field, the inelastic mean free-path li decrease and the electron becomes less located, and the resistivity of the system decrease.

The fitting parameters are α, H_φ and H_2. The best fitting is achieved with $H_2 = 0$. We find $H_\varphi = H_i = aT^p$ (see the insert in figure 3), with $a = 0.726$ and $p = 1.2$. This means that there are not contributions to the electron scattering by magnetic impurities (H_s=0) or spin-orbit coupling (H_{so}=0) and that the important mechanism is the inelastic scattering. The parameter values of the magnetoresistance are shown in Table I.

Table I
Fitted parameters of the transverse magnetoresistance of the layered compound $CuFeTe_2$

T(K)	R_s (Ω)	α	H_φ (Tesla)	L_{Th} (Å)
1.8	1.29x10^6	0.65	1.429	107
4.2	947520	0.82	3.869	65
20	354240	1.16	23.803	26

The effects of weak localization in two dimensions appear if the thickness *d* of the metallic sheets is much smaller than the Thouless length L_{Th}, which is related to the characteristic field H_i by the expression[12]

$$H_i = \frac{\hbar}{4eL_{Th}^2} \qquad (6)$$

The values of L_{Th} are indicated in the table 1. We can see that $L_{Th} >> d$ (d = 2Å according to the layered structure shown in figure 1), therefore it is reasonable to consider the $CuFeTe_2$ as an almost-2D system in relation to the electronic localization phenomena.

The T^p behavior of H_i has been observed in many disordered systems, such Au_xSi_{1-x}/Si (with p=2) and Cu/Si[13] multilayers, as well as in metallic thin films of Cu[14], Ag or Ag-Pd. Another case is the organic conductor $(DMtTSF)_2BF_4$, isomorphous to the Bechgaard salts (SDW systems), in which there were found effects of weak localization with $H_i \propto T$ (p ~ 1) [15]. In $CuFeTe_2$ we found p = 1.2. The value of p depends on the inelastic scattering mechanism at low temperatures. For the electron-phonon interaction p = 5, while for the s-d electron-electron interaction, p = 2. However, in metals with nesting in the Fermi surface a linear T scattering has been found[16], this could be the case of $CuFeTe_2$, in agreement with the SDW state.

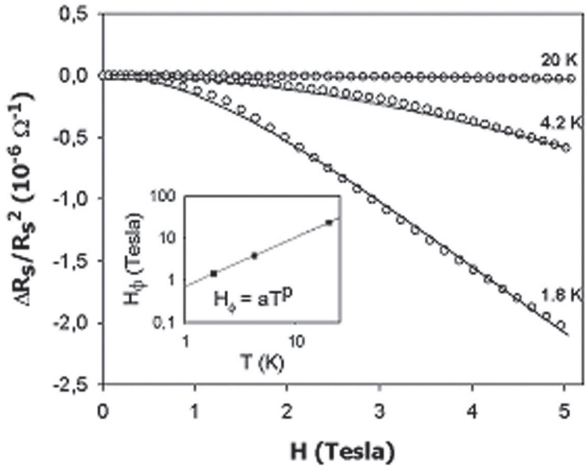

Figura 3. Transverse magnetoresistance of the $CuFeTe_2$. Insert: caracteristic field $H\varphi$ as a function of temperature.

CONCLUSIONS

The study of the electronic conduction at low temperature (down to 1.8 K), low current and high pulsed magnetic fields, performed for the first time on the layered compound $CuFeTe_2$, indicates the presence of weak localization in the cation planes of the almost-2D structure, being the interactions between conduction electrons the fundamental mechanism of inelastic scattering. Between 20 and 100 K the conduction is of hopping type assisted by phonons, without thermal activation of the carriers. Above 100 K the behavior of the resistance is attributed to the decrease of the fraction of electrons condensed in the SDW state.

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