HEAT CAPACITY AND PHASE TRANSITIONS IN A QUASI TWO-DIMENSIONAL SINGLE CRYSTAL $Cu_{1.04}Fe_{1.12}Te_{1.84}$

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The heat capacity of the quasi-dimerous sample $Cu_{1.04}Fe_{1.12}Te_{1.84}$ (CFT) obtained by the directional crystallization was experimentally studied in the temperature range 2–306K. On the temperature dependence of the C_p/T, a sharp maximum was revealed with T_G=55K, associated with the contribution of the spin-glass state, and the blurred anomaly was revealed near T_N=65K, due to the phase transition of the antiferromagnetary paramagnetic. The experimental results obtained are explained within the framework of a well-known model. From the experimental temperature dependence of the heat capacity of $C_p(T)$ CFT (copper of iron television), the debye temperature is calculated Θ_D=176.9 K, as well as the anisotropy coefficient η=0.309 and the two-dimensional temperature of the debt Θ_2=122.2K.

Keywords: heat capacity, quasi-humid, spin-glass, antiferromagnetik.
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1. INTRODUCTION

As a reason for the manifestation of superconducting properties in iron chalcogenides, varies from the standard BKSH mechanism to the magnon mating, which freshen the effect of antiferromagnetic exchange interactions or the effect of non-varic fluctuations that suppress magnetic ordering in the system. Recently, a single opinion is begining to form about the dominant effect of non-varicing ordering crystals and its relationship with spin fluctuations in the FeCh system (S, Se, Te). The study of the dynamics of the lattice of quasi-minor magnetic materials gives information that reflects nature and characterizes changes in intra and interlayer interactions, based on which various microscopic models can be built. Below, we consider experimental tests of the heat capacity of the quasi-duty antiferromagnetic compounds $Cu_{1.04}Fe_{1.12}Te_{1.84}$≈$Cu_{1.13}Fe_{1.22}Te_2$ (in the long-term short CFT) temperature areas of spin-glazing conditions and the magnetic phase transition of the antiferromagnetary paramagnetic.

The temperature dependence of the heat capacity of the CFT single crystal was investigated in the temperature range 2-306K by the authors [1].

The aim of this work is to study the features of the magnetic, lattice, and phase transitions of the $Cu_{1.04}Fe_{1.12}Te_{1.84}$ compounds based on the experimental data on the specific heat in the temperature range 2-306K.

2. OBJECTS OF RESEARCH AND EXPERIMENTAL TECHNIQUE

Unsticiometric CFT single crystals were synthesized and the electrical, magnetic and effect of Mossbauer in the works [2-8].

X-ray analysis of CFT crystals grown with tetragonal symmetry with elementary cell parameters A=3.97±0.004Å, C=6.11±0.004Å and V=96.2991Å^3, spatial group P4/nmm, Z=1, ρ=6.5g/cm^3. These data coincide with [2-8], as well as an identical spatial group of $Fe_{1+\delta-X}Cu_XTe$ compounds [9] and $Fe_{1.1-Z}Cu_ZTe$ [10]. To establish the nominal composition of single crystals and clarifying their crystal structures, an analysis of the compositions in the EDX type analyzer (Energy Dispersive X-Ray Analysis) was carried out and duplicated by analyzing Analyst-800 Perkin Elmer. Automatically calculated atomic percentages corresponded to the following values for CFT single crystals: Cu=18.18 ± 1.85; Fe=17.21 ± 1.86; Te=64.61±2.27. The crystal structure is a defective structure of the Cu_2Sb type, which is identical to the Ricarditis structure - $Cu_{2-X}Te$, but with additional nodes between Cu/Fe - Tetrahedron (fig. 1).

The structural formula of the chalcopyrite type single crystals corresponds to: $Cu^+ Fe^{3+} Te_2$ ($Cu_{0.04}$ and $Fe_{0.12}$) due to the lack of Tellur Anion ($Te_{0.16}$) appear "surplus" atoms Cu^{2+} and Fe^{2+} are chaotic located in the voids of the crystal lattice and behave as impurities (nanoparticles) [3, 8].

In layered crystals, the interatomic interaction leads to unusual temperature dependences of heat capacity with specific fiction laws at low temperatures [11-13]. The same was observed in anisotropic layered magnets, where phase transitions are fluctuation in nature [14-16].

The $Cu_{1.04}Fe_{1.12}Te_{1.84}$ heat capacity was measured in the 2-306K intervals on the Quantum Design PPMS commercial device (Physical Property Measurement System) [1].

In [1], the dependence of the characteristic temperature of the Debye $\Theta_D(T)$ for $Cu_{1.04}Fe_{1.12}Te_{1.84}$ is calculated. Analysis of the Debye and Einstein model theoretical approaches used to describe the lattice part of the crystal heat capacity. The temperature changes of the entropy ΔS are calculated.

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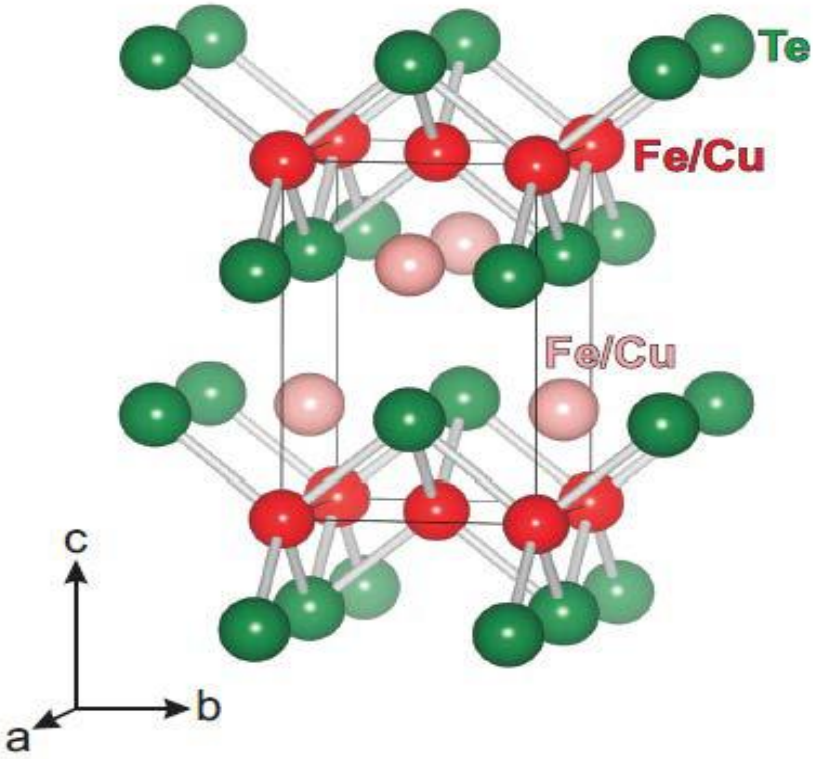

Fig. 1. Cu and Fe atoms (labeled in red) occupy 2A (0 0 0) nodes, with filling of about 50% for each of these atoms, and Te atoms (marked with green) nodes 2c (0 1/2 Z). Additional nodes in [2c '- (0 1/2 z')] (marked with pink color) were partially filled with Cu and Fe atoms with a filled with less than 15% [8]

3. EXPERIMENTAL RESULTS AND THEIR DISCUSSION

In fig. 2 shows the results of measuring the temperature dependence of the heat capacity (Cp) and the excess component of the heat capacity of C_{pexs}-C_{pD}=ΔC_p(T), where C_{pexs}-experimental results and C_{pD}-the calculated lattice value of the heat capacity in the Debye model [1].

The linear portion of $C_p(T)$ covers the temperature range from 65 to 125K (see fig.2 $\Delta C_p(T)$), the ΔC_p *curve* (T) undergoes the breaking at the temperature of the antiferromagnetic T_N=65K and the spin-glazing conversion T_G=55K.

The dependence $\Delta C_p(T)$ clearly shows when ΔC_p=0 Phase transitions spin-glazing (T_G=55K) and antiferromagnetic paramagnetic (T_N=65K).

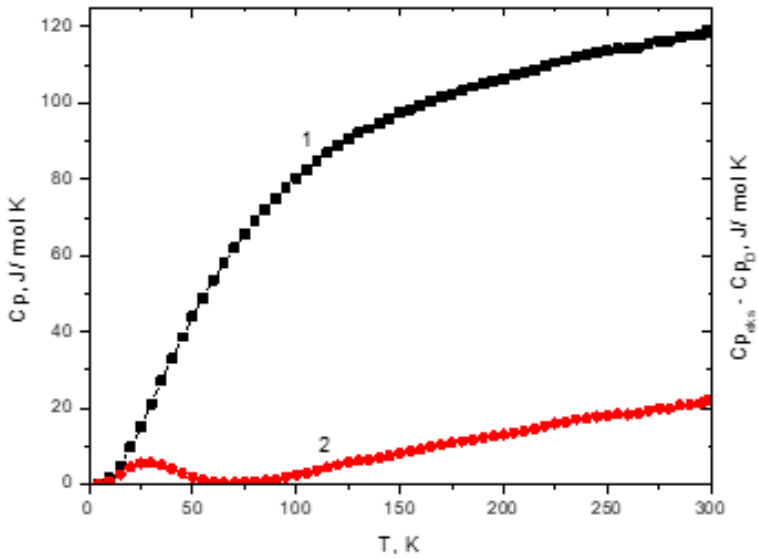

Fig. 2. Temperature dependences of heat capacity: 1- C_p heat capacity and 2-(C_{pexs}.-C_{pD}) excess component of the heat capacity of the CFT connection. C_p and C_{pexs} - experimental importance, and C_{pD} - calculated lattice value of heat capacity in the Debye model ($C_{pD}= 9Nk_B{\cdot}T{\cdot}\left(\frac{T}{\theta_D}\right)^3 \int_0^{\frac{\theta_D}{T}} \frac{x^4 e^x}{(e^x-1)^2}$ dx; $x= \hbar\omega/k_BT$)

In [14], the "blurring" of the transformation near the transition temperature with a slightly different point of view is discussed. Those. Sets the identity between phase transitions of the second kind and critical phenomena. Near the magnetic conversion temperature due to the development of fluctuations (because the thermodynamic potentials of both phases are close in size) there is a bundle of a homogeneous phase into a large number of "groups" of spins forming a magnetic dispersion system. As the phase transition is removed from the point or down, the dispersion decreases, and the system becomes homogeneous. The presence of this dispersion in the phase transition region and causes the "blur" of the maximum on the temperature curve of the heat capacity. The advantages of the exact use of the principles of thermodynamic stability are particularly clearly manifested when analyzing the data obtained under conditions of low temperatures.

Kinetic energy at low temperatures is small; therefore, the course of the dependences of $C_p(T)$ and $C_p/T(T)$ will become completely different. In the field of low kinetic energy, "blurred" phase transitions are possible, due to small changes in potential energy, which are detected when constructing C_p/T from T [15]. The point of view of the work [15] essentially coincides with the theoretical position of [14], but in an implicit form it is used by the concept of fluctuations of far magnetic order [16,17].

Given the unusual character of the magnetic phase transition to CFT on the basis of the experimental data of the $C_p(T)$, the temperature dependence of C_p/T was constructed [17].

Dependence of C_p/T from T fig. 3 shows unusual (diffusion [14], blurred [15] and fluctuation [16]) the nature of the phase transition.

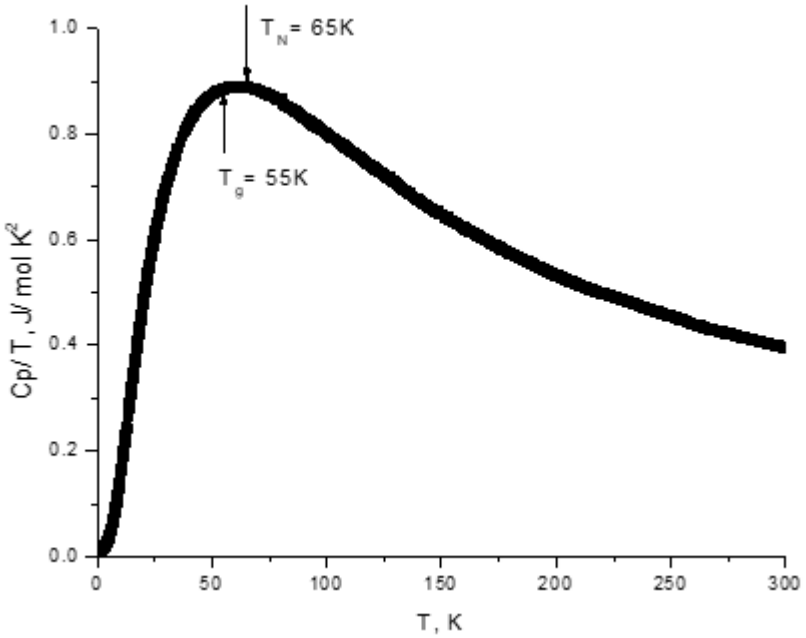

Fig. 3. Temperature dependence of the heat capacity of C_p/T from T.

In fig. 3a presents the results of the processing of the experimental data according to the method described in [13], in the coordinates of $C_p/3n_0Nk_B$-T/Θ_D, where n_0=4 is the number of atoms in the molecule of the crystal under study, $3Nk_B=R$ is the gas constant, N is the number of Avogadro, k_B-Boltzmann Constant, Θ_D-Debye temperature. In the same figure (fig. 3b), the dependence of C_p/T from T^2 (cubic law Debye) is within T/Θ_D

$$C_{lat} \rightarrow \beta \cdot T^3 = 12\,\frac{R\pi^4}{5}\cdot(T/\theta_D)^3 \qquad (1)$$

From the experimental data, the Debye temperature was calculated using the formula Θ_D = (1942.7 $\frac{n_0}{\beta}$)$^{1/3}$ (where n_0 = 4 is the number of atoms in the molecule of the crystal under study, β=1.404mJ·mol^{-1}·K^{-4}, Θ_D=176.9 K - Debye temperature at T→0 K [12]). This suggests that structural anisotropy in the compound does not affect the behavior of the heat capacity below 15.1K.

To determine the anisotropy parameter η and a two-dimensional debit temperature Θ_2 in CFT, an equation is used characteristic of layered crystals with a linear section of temperature dependence [13].

$$C_p/R = \pi^2 T/\theta_2(1-\eta) - \eta/(1-\eta) \qquad (2)$$

Where

$$\Theta_2 = \pi^2 R\,/3(1-\eta)\,\partial C_p\,/\partial T,\ \eta = \Delta C_p\,/1+\Delta C_p$$

From fig.3a it is not difficult to estimate η=0.309 and Θ_2=122.2K ($Cp/3n_0k_BN$ = -0.448 at T=0) and η=0.309, and Θ_2 =(1-η) Θ_D=122.2K.

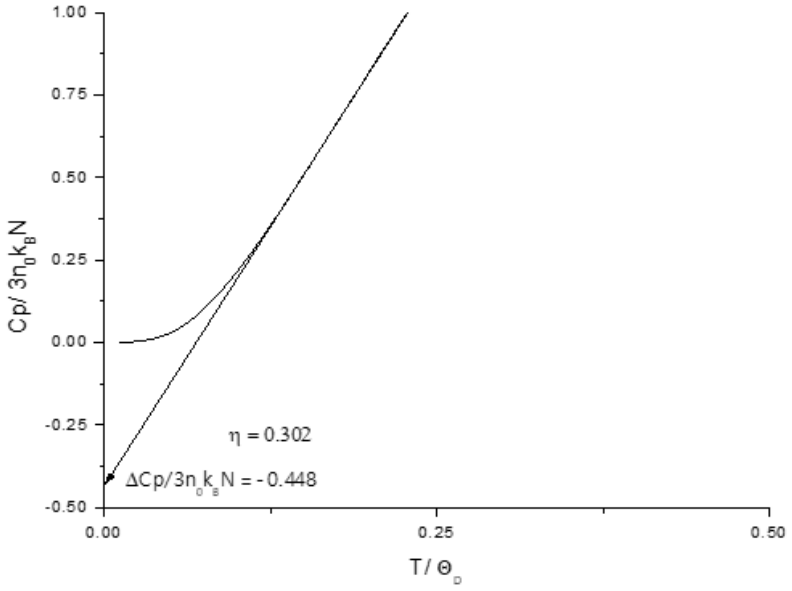

Fig.3a. Dependence of heat capacity from temperature in coordinates $C_p/3n_0k_BN$ -T/θ_D.

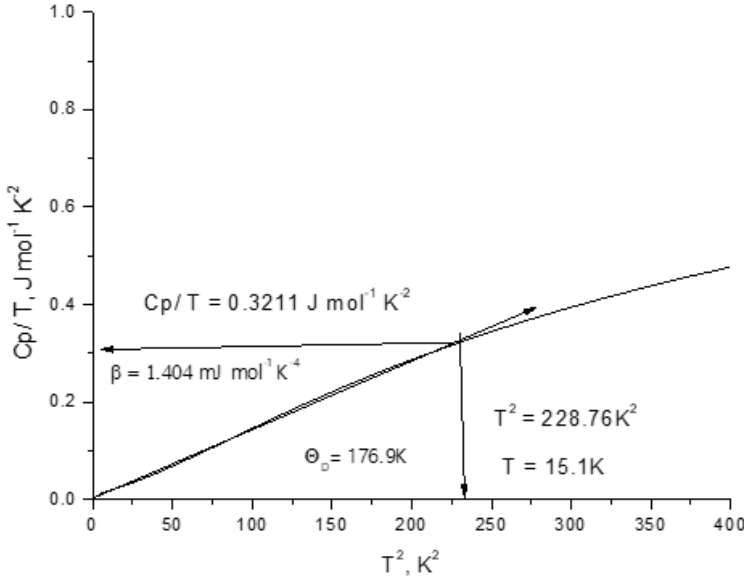

Fig. 3b. C_p/T from T^2 cubic law Debay

4. CONCLUSION

1. The linear section of the temperature dependence of the heat capacity in the range 65-125K indicates the quadratic dispersion law and is mainly due to the additive contribution of bending and spin waves.
2. Detected spin-glazing (T_G = 55K) and antiferromagnetic (T_N=65K) Phase transitions are characterized by a temperature, intake on the C_p/T dependence on T, which is characteristic of quasi-humid materials.
3. Anisotropy parameter η=0.309, Debye temperature Θ_d=76.9K and 2D-temperature Debye Θ_2 122.2K.

The values of heat capacity for $Cu_{1.04}Fe_{1.12}Te_{1.84}$, change entropy, enthalpy and the reduced free energy of Gibbs at a temperature of 298.15K.

T, K	*Cp, J/ mol K*	$S_T - S_0$, *J/ mol K*	$H_T - H_0$, *J/ mol*	$-\Delta F$, *J/ mol K*
298.15	118.594	178.26	24772	- 28379

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