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Resistivity of Graphite Intercalation Compounds with Bromine and Aluminum Chloride under the Pressure

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The paper presents the results of investigation of resistivity of acceptor graphite intercalation compounds in the temperature region of phase transition in the intercalate layers. The features of phase transitions in intercalate layers under pressure and temperature are found. It is shown that the resistivity of graphite intercalation compounds increases under pressure, the temperature of phase transformations in the intercalate layer shifts to higher temperatures. Parameters of the electronic structure of graphite intercalation compounds and their pressure dependence are estimated. Changes in the resistivity of graphite intercalation compounds under pressure are calculated.

Keywords: Graphite intercalation compound, Resistivity, Phase transition, Layer of intercalate

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1. INTRODUCTION

The present level of science and technology provides great opportunities for creation of new functional materials, among them different types of composites, including layered composites.

A characteristic feature of layered materials is an anisotropy of properties, particularly, a significant difference of binding energy for atoms belonging to one layer and atoms of different layers. One of the most promising materials with a strong anisotropy of the properties along the layers and perpendicular to the layers is graphite. Graphite materials (natural dispersed graphite, thermoexfoliated graphite, graphite fibers etc.) are widely used as fillers at the creation of various composite materials. Graphite also due to its clearly expressed structural anisotropy is the basis for obtaining of layered composites - graphite intercalation compounds (GICs). When monomolecular or monoatomic layers are introduced into the graphite interplanar space, the distance between the layers of graphite increases by several times in comparison with the source matrix. The new periodic structure (GIC) thus is formed, in which the graphite layers are alternated with layers of intercalate. GICs are characterized by stage number S (number of graphite layers between the nearest monoatomic or monomolecular layers of intercalate) and identity parameter I_s (distance between adjacent layers of intercalate).

GICs are natural two-dimensional electronic systems in which carriers move mainly in the parallel to the graphite planes direction. During intercalation process there is a charge transfer from intercalates molecules to graphite layers, and layers of graphite are enriched with additional charge carriers. In this process halogens and halides act as electronic acceptors, enriching the graphite layer with additional delocalized holes. A number of physical phenomena, experimental observations of that in other materials are significantly complicated, have been investigated in GICs [1-3]. Among these phenomena there are phase transformations in two-dimensional systems and their effect on the transport properties of GICs. Structural peculiarities of phase transformations in GICs based on HOPG and fine-crystalline graphite with iodine and stibium chlorides under the temperature and pressure quite well studied [4]. However, the properties of these compounds with other halogens and halides, such as, eg, aluminum chloride and bromine, studied much less.

The investigation of transport properties GICs under pressure allows to estimate the dependence of their electron structure parameters from pressure, to detect the regularities of phase transitions in the intercalates layers and to create adequate model of phase transitions in low-dimensional systems.

The aim of this work is to study the resistivity of acceptor GICs and to reveal the influence of temperature and pressure on the conductivity mechanisms and electronic structure parameters of GICs.

2. OBJECTS AND METHODS

In the work investigations of the resistivity ρ_a along the graphite planes depending on temperature and pressure were carried out for specimens of GICs based on fine crystalline pyrolytic anisotropic graphite (FPAG) with aluminum chloride and bromine. The crystalline structure parameters of source for intercalation FPAG are: distance between neighboring graphite layers $d = 0.340$ nm, crystallite size $L_b = 20$ nm, the parameter of crystallites preferred orientation $h = 10^3$.

GICs specimens were obtained with standard two-temperature gas-phase method. The stage S of obtained compounds was determined by X-ray diffraction data. Intercalation process parameters (temperatures of graphite T_{gr} and intercalate T_{int} and intercalation time t) and stage of compounds S are shown in Table 1.

As it is shown from the Table the specimens of second stage GICs with aluminum chloride and bromine were obtained. GICs specimens for measuring of

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Table 1 – Synthesis temperature and time and stage of GICs

N	Intercalate	T_{gr}, K	T_{int}, K	*t*, hrs	*S*
1	$AlCl_3$	483	483	48	2
2	Br_2	318	318	48	2

transport properties were cut in the form of rectangular parallelepipeds with size 2 mm × 3.5 mm × 15 mm. The measuring of transport properties of GICs was carried out by standard four-probe method [8]. High hydrostatic pressure chamber was used for measuring of electrical resistance of specimens under pressure. The resistivity was investigated in the temperature interval from 77 K up to 293 K and under the pressure up to 1.2 GPa. Resistance measurement error does not exceed 0.05 %.

3. EXPERIMENT

3.1 Experimental Dependence of Resistivity from Temperature

Figure 1 presents the typical temperature dependence of resistivity $\rho_a(T)$ for specimens of GIC with bromine at different cooling and heating rates.

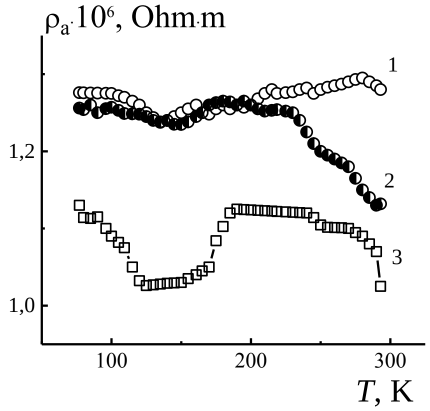

Fig. 1 – The dependencies $\rho_a(T)$ for GIC with bromine: 1 – rapid cooling (2 K/min), 2 – rapid cooling after exposure at $T = 77$ K for 12 hrs. (2 K/min.), 3 – exposure at $T = 77$ K, cooling after rapid heating (2 K/min.)

As seen from Figure 1, at the initial rapid cooling of the specimen (curve 1) there are a very weak dependence of resistivity on temperature with a slight decrease of resistivity with temperature decreasing and poorly pronounced minimum at 140 K. Exposure of the specimen during 12 hours at 77 K does not lead to change of the resistivity. At fast heating of the specimen (curve 2) view of the temperature dependence of resistivity coincides with a view of the resistivity temperature dependence at cooling, but at the temperature above 220 K the resistivity is reduced by ~ 15 % compared with the initial value. The exposure of specimen at 77 K within five days results in a further decrease of the resistivity and a pronounced minimum in a $\rho_a(T)$ dependence is observed in temperature range from 100 K to 180 K.

Figure 2 presents the typical temperature dependence $\rho_a(T)$ for GIC specimen with aluminum chloride.

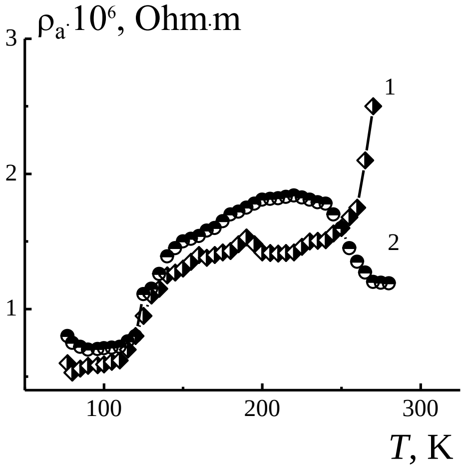

Fig. 2 – The dependencies $\rho_a(T)$ for GIC with aluminum chloride:1 – slow cooling (0.5 K/min.), 2 – exposure at $T = 77$ K, slow heating (0.5 K/min)

As it is shown from Figure, for GICs with aluminum chloride metallic character of temperature dependence of resistivity $\rho_a(T)$ is observed, that is typical for low stage GICs with polar intercalates. The resistance temperature coefficient (RTC) is $4.4 \cdot 10^{-3}$ K^{-1}, which is close to the value of RTC in metals. However, $\rho_a(T)$ is not monotonic. When the temperature decreases from 293 K to 250 K ρ_a value is reduced by half. At temperature (180-220) K weak vague minimum is observed. With further decreasing of temperature resistivity continues to decrease to a value ~ 5 10^{-7} Ohm m at the temperature of liquid nitrogen. At the heating there is a similar view of the temperature dependence of $\rho_a(T)$, but local minimum in the dependence $\rho_a(T)$ is observed at significantly higher temperatures.

3.2 Experimental Dependence of Resistivity under Pressure

The investigations of resistivity dependences from pressure $\rho_a(P)$ at constant temperature and from temperature $\rho_a(T)$ under constant pressure for specimens of GICs were carried out.

The typical dependence $\rho_a(P)$ at room temperature for cycle loading – unloading for GIC with bromine is presented on the Figure 3.

As it follows from Figure, for GIC with bromine very weak dependence $\rho_a(P)$ at room temperature is observed, and dependence is not monotonic.

Figure 4 presents the typical dependences $\rho_a(T)$ for GIC with bromine under constant pressure.

As seen from Figure, under hydrostatic pressure 1.2 GPa resistivity ρ_a at room temperature increasei in 1.6 times in comparison with unloading specimen. As the temperature decreases, the resistivity ρ_a decreases very slightly, in the temperature interval (175-225) K there is a weakly pronounced vague minimum in $\rho_a(T)$. At the heating of specimen from 77 K to 293 K the view of the temperature dependence $\rho_a(T)$ is practically coincide with the view of temperature dependence $\rho_a(T)$ at cooling. Upon removal of the load the value ρ_a at room temperature is increased by 1.5 times compared

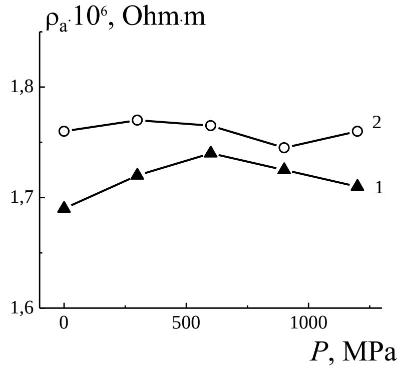

Fig. 3 – The dependencis ρa(*P*) at *T* = 293 K for GIC with bromine: 1 – loading, 2 – unloading

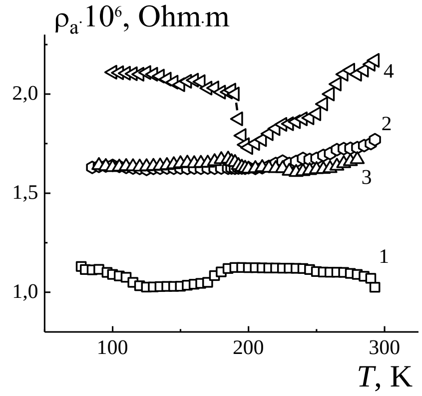

Fig. 4 – The dependencies $\rho_a(T)$ for GICs with bromine under constant pressure: 1 – before loading, cooling, 2 – $P = 1.2$ GPa, cooling, 3 – $P = 1.2$ GPa, exposure during 24 hours at $T = 77$ K, heating, 4 – after removing the load, cooling

to the loaded specimen. At cooling the specimen after removal of the load the temperature dependence $\rho_a(T)$ is identical to the $\rho_a(T)$ in the specimen under load, but minimum in the temperature range (175 – 225) K has a pronounced character.

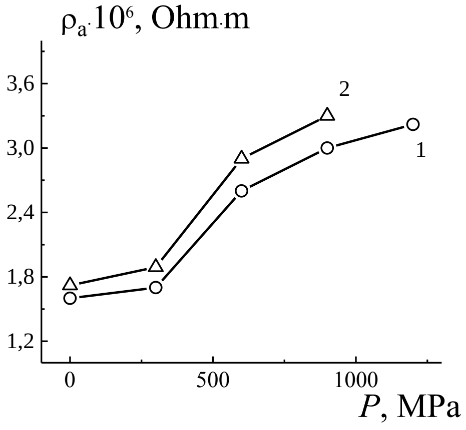

Fig. 5 – The dependencies $\rho_a(P)$ at $T = 293$ K for GIC with aluminum chloride: 1 – loading, 2 – another specimen, loading

The typical dependence $\rho_a(P)$ at room temperature for GIC with aluminum chloride is presented on the Figure 5.

As it is shown from Figure, significant dependence $\rho_a(P)$ is observed. With increasing load up to 1.2 GPa ρ_a value increases significantly (to two times).

4. DISCUSSION

As it is known, phase transformations in the intercalates layers lead to the appearance of abnormal temperature dependences of the kinetic properties in the GICs. In particular, in the temperature dependence of resistivity at temperatures, at which there are phase transitions in the intercalates layers, local extremes, changes in the slope of dependencies, sharp rise in the value of electrical resistance are observed [5].

Let us consider the factors, that can lead to the change of the electrical resistance of GIC in the temperature region of phase transition in the intercalate layer. These factors are:

- change in the state density at the Fermi level $N(E_F)$ at phase transition, that is directly linked with the share of charge *f*, which is transmitted from one intercalate molecule to graphite layers;
- the changing of character of carrier scattering, ie the change of carriers effective relaxation time t_{ef} caused by a change in the phonon spectrum due to restructuring of intercalate layer. In the process of restructuring there are changes in the ordering of intercalates molecules in the layer. That is, the transition from one type of intercalate ordering to another occurs. For example, these are transitions from noncommensurate to commensurate two-dimensional lattice or transition from "quasicrystalline" to "quasiliquid" state;
- the change of electrical resistance of intercalate layer.

The temperature dependence of the resistivity of low stages GICs at temperatures below the phase transition temperature in the intercalate layers is caused by the temperature dependence of charge carrier scattering mechanisms, because charge carrier concentration in these compounds is almost independent of temperature. Intercalate layer is a two-dimensional ion crystal, electrical resistivity of which is several orders higher, than the resistivity of graphite layers. GICs conductivity is determined mainly by conductivity of enriched with additional charge layers of graphite. Any structural transformation in the intercalate layers, at which the transition from one "quasicrystalline" structure to another occurs, if it does not change the composition of the intercalate ions, does not lead to changes in accommodation coefficient *f*, but changes the value of the charge carriers mobility. Such change of charge carrier's mobility is caused by the changing of the effective relaxation time at charge carriers scattering on graphite and intercalate phonons. If in the intercalate layer there is transition from "quasicrystalline" to "quasiliquid state", in this case intercalate is a "mobile ions liquid" that fills the space between two graphite layers. When a constant electric field is applied or when there is a temperature gradient, in GIC movement or orientation redistribution of intercalate ions can occur that cause their uneven distribution. Volumetric charge accumulated in the contact area that leads to changes in the effective conduction of layer. That relaxation ion-migration polarization occurs.

Let us analyze in the terms of present model changes in GICs resistivity in the phase transitions region in depending on pressure and temperature. It is known, when in the interplanar space of graphite acceptor intercalate is introduced, in the substance-intercalate disproportionation reaction occurs. As result of disproportionation reaction neutral molecules of intercalate are converted into negative ions, and layers of graphite enriched with additional carriers - holes. Intercalate ions form depending on the character of interaction between them and graphite layers a commensurate or incommensurate two-dimensional lattices. For example, aluminum chloride polar molecules, when they are introduced into graphite, according to the disproportionation reaction $AlCl_3 + e^- \rightarrow AlCl_4^-$ are converted to anions. The anions $AlCl_4^-$ form commensurate with the graphite layer two-dimensional lattice. The situation is more complex with intercalation of non-polar halogens molecules in graphite. X-ray diffraction data indicate that the introduction of non-polar halogens molecules into graphite results in formation of layered structure with periodic placement of graphite and intercalate layers up to the first stage [6].The change of the value of resistivity of GICs with non-polar intercalate indicates, that the charge transfer from intercalate molecules to the graphite layers occurs. That is non-polar halogen molecules during intercalation process are polarized.

One of the nonpolar intercalates, structural phase transitions for which are intensively studied, is bromine. As shown in the literature [7], in layers of bromine there is a number of structural transformation associated with different ordering of bromine in layer. Thus, for second stage intercalated compounds based on highly ordered pyrolytic graphite (HOPG) three phase structural transitions are known: at 240 K transition from one commensurate "quasicrystalline" to another commensurate "quasicrystalline" phase, at 333 K transition from commensurate to incommensurate "quasicrystalline" phase, and at 373 K transition from "quasicrystalline" phase to "quasiliquid" phase [8]. Thus, in the temperature range under study, there is only one structural phase transition, which is not associated with melting of the intercalate lattice. However, as shown in recent studies of phase transitions features for GICs with non-polar intercalate, in these compounds variation of accommodation coefficient *f* in some phase transitions, such as commensurate "quasicrystalline" to another commensurate "quasicrystalline" phase, is observed. This transition in the bromine layers for based on HOPG GIC occurs at 240 K.

Thus, for GICs with polar intercalate (aluminum chloride) structural phase transitions do not lead to changes in the charge share, transferred from intercalate molecules to graphite layers, and, therefore, do not change the states density at the Fermi level $N(E_F)$. For those GICs resistivity change is associated only with the change of charge carrier's effective relaxation time.

Let us consider the resistivity of acceptor GICs in terms of two-dimensional electron structure model [9]. In this model two-dimensional resistivity for the second stage GIC can be written as the sum of two terms:

$$\rho = \rho_{2S_0} + \rho_T , \tag{1}$$

where ρ_{2S0} is the temperature independence term and ρ_T is the temperature dependence term. The temperature independence term or residual resistivity can be written as

$$\rho_{2S_0} = \frac{\pi h}{e^2 k_F} \cdot \frac{1}{L_b} , \tag{2}$$

where L_b is the charge carriers mean free path at the scattering on the crystallites boundaries, k_F is the Fermi wave vector.

The temperature dependence term is written as:

$$\rho_T = \frac{\pi h}{e^2 k_F} \cdot \frac{1}{L_T} , \tag{3}$$

where L_T is the charge carriers mean free path at the temperature dependence scattering mechanisms.

Consider the main charge carrier scattering mechanisms that lead to the appearance of the temperature dependence of the relaxation time and consequently that form temperature dependence of resistivity in GICs.

First, this is electron-electron scattering, which leads to quadratic temperature dependence of resistivity [10]. However, according to estimates, resulted in a number of works for the second stage GICs with SbF_5 [10], the charge carriers mean free path at carriers scattering each other is $7 \cdot 10^{-5}$ m at 100 K. This value is significantly higher than the mean free path at the scattering of charge carriers on phonons and crystallites boundaries. Secondly, this is charge carrier scattering on phonons, which includes scattering on the different modes of graphite and intercalate.

Thus, in a first approximation summarized temperature dependence of the charge carriers mean free path is determined by the temperature dependence of the mean free path for scattering on phonons, as at other temperature-dependent scattering mechanisms mean free path is much larger: $L_T = L_{ph}(T)$. Charge carriers mean free path at the scattering on phonons is inversely proportional to temperature and can be written as:

$$L_{ph} = L_0 T^{-c} , \tag{4}$$

where L_0 is the constant.

Thus, the two-dimensional resistivity for second stage GIC in terms of electron structure two-dimensional model can be written as:

$$\begin{aligned} \rho_{2S} &= \frac{\pi h}{e^2 k_F} \cdot \left(\frac{1}{L_b} + \frac{1}{L_{ph}(T)} \right) = \\ &= \frac{3\pi h b \gamma_0}{2e^2 E_F} \left(\frac{1}{L_b} + \frac{1}{L_{ph}(T)} \right) \end{aligned} , \tag{5}$$

where E_F – is the Fermi energy, *b* is the distance between neigboring carbon atoms in graphite layer, γ_0 is the interaction energy of neigboring carbon atoms in graphite layer.

Since the charge carriers effective relaxation time at the scattering on the crystallites boundaries is constant for GIC based on certain graphite material, the resistivity of GICs with polar intercalate at the phase transition region can be changed only due to changes of charge carriers relaxation time at the scattering on the phonons, in particular, scattering on the graphite phonons t_{ph0} and the intercalater phonons t_{phi}. According to [11] $(t_{ph0})^{\square-1}\sim(\square q_0)^2$, where $q_0=1/(\gamma_0(\partial\gamma/\partial r))$; $\partial\gamma/\partial r$ characterizes the change in the interaction of atoms with changing the interatomic distance r. This value depends also on how the intercalater molecules are distributed in layer, as they induce a charge in the graphite layers.

Value $(t_{ph})^{-1}$ depends on the charge density fluctuations in the intercalate layer, which in turn affects on the screened charge in the intercalate layer. The changing of the distribution of molecules in the intercalate layer obviously leads to the changes in the value $(t_{ph})^{-1}$ and its temperature dependence. Changing of the type of the carriers relaxation time temperature dependence results in change in slope of the curve $\rho_a(T)$. However, as shown in number of studies, for example [1], the relative contribution to the resistivity due to carrier scattering on the phonons essentially depends on the structure peculiarities of the source for intercalation graphite. For GICs based on structurally imperfect forms of graphite (FPAG) preferred carrier scattering mechanism is a scattering on the crystallites boundaries. For GICs based on such graphite materials the relative change of resistivity in the phase transition temperature interval is less pronounced in comparison with GICs based on perfected graphite (HOPG), for which the charge carrier scattering on the phonons is more significant. Note that the phase transition temperature in the GIC-based on FGPG with bromine is reduced in comparison with the same temperature in the GIC based on HOPG. From obtained experimental data it follows that the phase transition temperature T_{tr} for GIC based on FPAG is = 160 K, while for GIC based on HOPG T_{tr} = 240 K. As shown in [5], the use of the fine crystalline graphite with a relatively weak interaction between graphite layers as source graphite for intercalation leads to the formation of GICs with greater identity parameter I_s. This is equivalent, in a first approximation, to reducing of pressure along the axis C. Estimation of temperature shift, is carried out under the assumption, that increasing of the distance between the graphite layers in the FPAG is equivalent to decreasing of the external pressure, gives the value ~ 80 K. This value well corresponds with the experimental obtained value of the phase transition temperature in the GIC based on FPAG: 240 K – 80 K = 160 K. Results of experimental studies of the temperature dependence $\rho_a(T)$ at constant pressure also confirm these calculations. As follows from the experimental data (Fig. 4) applied hydrostatic pressure 1.2 GPa to the specimen of GIC with bromine shifts the phase transition temperature on 40 K in upward temperature.

Let us estimate in the terms of two-dimensional model of the electronic structure (equation (5)) with using the experimental data on dependence $\rho_a(T)$ values of the Fermi energy for studied GICs. Estimated values of the Fermi energy are: for GIC with $AlCl_3$ E_F = 0.514 eV and for GICs with bromine E_F = 0.377 eV.

As follows from the experimental data of the study of resistivity ρ_a on pressure, increasing the pressure at constant temperature does not cause the increasing of resistivity (GIC with bromine) or causes slightly increase (GIC with aluminum chloride). This result is unexpected, although it is fully correlated with data on pressure dependence of resistivity for based on HOPG GICs with antimony chloride [12].

Let us consider in detail the pressure dependence of the resistivity along the planes of graphite $\rho_a(P)$. At high temperatures it is possible according to [24, 25] to write the expression for ρ_a:

$$\rho_a \propto \frac{T\lambda_{e-ph}}{\omega_{pl}^2}, \qquad (6)$$

where ω_{pl} is the plasma frequency, λ_{e-ph} is the electron-phonon interaction parameter, that can usually be calculated approximately from the Grüneisen parameter γ as $dlnl_{e-ph}/dp=-2gk$. This parameter can be determined in different way. Usually, the thermal average, calculated from specific heat, compressibility, and thermal expansion, is used. In [13**Ошибка! Закладка не определена.**] Grüneisen parameter for graphite has been calculated with using data on specific heat, compressibility, and thermal expansion. As have shown calculations, the value of γ essentially depends on the direction in graphite and $\gamma = -1$ in the plane of graphite layer and $g = 0.25$, if the average value on volume is determined. The pressure dependence of ω_{pl} can be written as [14]:

$$\omega_{pl}^2=\frac{8e^2}{\hbar^2 I_S}E_F\left[\frac{E_F^2-\frac{\gamma_1^2}{2}}{E_F^2-\frac{\gamma_1^2}{4}}\right]. \qquad (7)$$

where γ_1 is the interaction energy for nearest carbon atoms in neighboring graphite layers. For estimation of the plasma frequency ω_{pl} changes with the pressure necessary to determine how for studied specimens such parameters as identity parameter I_s, Fermi energy E_F and the parameter γ_1 are changed with pressure.

For estimation the pressure dependence of the interaction energy of neighboring layers of graphite γ_1 the results of the [15] have been used. According to [15] $\frac{\Delta\gamma_1}{\Delta p}=0.026eV\cdot GPa^{-1}$. The identity parameter I_s changing has been estimated with using the value $\frac{\Delta c}{c\Delta p}=2\cdot10^{-11}Pa^{-1}$ for pure graphite [16]. The pressure dependence of Fermi energy for GIC with bromine has been determined from obtained temperature dependences of resistivity at different pressure (Fig. 4) in the terms of two-dimensional electron structure model. For estimation of pressure dependence of the Fermi energy of GICs with aluminum chloride the data of work [16], which exhibits the experimental dependence $E_F = f(p)$ for GICs with polar intercalate, have been used. According to the experimental dependence $\frac{\Delta E_F}{\Delta p}=0.04eV\cdot GPa^{-1}$.

The Table 2 presents the results of estimation of parameters I_s, E_F and γ_1, and also calculated values of plasma frequencies ω_{pl}^2 in the absence of applied pressure and under hydrostatic pressure $p = 1.2GPa$.

Table. 2 – Parameters I_s, E_F, γ_1 , ω_{pl}^2 in the absence of applied pressure and under hydrostatic pressure p = 1.2 GPa for GICs with aluminum chloride and bromine

N	GIC – $AlCl_3$		GIC – Br_2	
	$p = 0$	p = 1.2GPa	$p = 0$	p = 1.2GPa
γ_1	0.390 eV	0.356 eV	0.390 eV	0.356 eV
I_s	1.286 nm	1.270 nm	1.038 nm	1.022 nm
E_F	0.514 eV	0.394 eV	0.377 eV	0.259 eV
ω_{pl}^2	$1.09 \cdot 10^{21}$	$7.26 \cdot 10^{20}$	$8.16 \cdot 10^{21}$	$8.37 \cdot 10^{19}$
$\frac{\rho_{a1.2}}{\rho_{a0}}$	~ 1.98		~10	
$\frac{\rho_{a1.2}}{\rho_{a0}}*$	~ 2		~(1.1 – 1.4)	

With the use of estimated parameters I_s, E_F, γ_1 according to formula (6) ratio of resistivity under the pressure 1.2GPa and in the absence of pressure $\frac{\rho_{a1.2}}{\rho_{a0}}$ were calculated. The values of these ratios also are given in Table 2. For comparison, in the table also ratio of experimental values of resistivity in the absence of pressure and under pressure 1.2 GPa $\frac{\rho_{a1.2}}{\rho_{a0}}*$ are presented.

As the table shows, for GICs with aluminum chloride very good coincidence between the calculated and the experimental values of $\frac{\rho_{a1.2}}{\rho_{a0}}$ is observed. As for the GICs with bromine, for this compound calculated and determined experimentally resistivity ratio $\frac{\rho_{a1.2}}{\rho_{a0}}$ differ nearly 10 times. Such differences may have related to the fact, that in the GIC with bromine under pressure there are structural phase transitions in layers intercalantthat, that lead not only to the change in the coefficient of accommodation due to changes in polibromine chains structure, but also cause the change in the nature of interaction between the graphite and intercalate layers and, as a result, significantly alter the electron-phonon interaction.

5. CONCLUSIOS

As a result of experimental research of temperature and pressure dependences of resistivity it has been found:

1. Anomalies in the temperature dependence of resistivity in the temperature region of phase transition in the intercalate layer are revealed.
2. The shift of the phase transition temperature in GICs based on fine-crystalline graphite in comparison with GICs based on high oriented graphite is found.
3. It is shown that the under applied pressure the temperature of phase transition in specimens of GICs based on fine-crystalline graphite shifted toward higher temperatures. And resistivity change in the phase transitions temperature region in the specimens under pressure is significantly lower than in the specimens in the absence of applied pressure.
4. In the terms of two-dimensional electron structure model the Fermi energies and their pressure dependences for GICs with aluminum chloride and bromine are estimated.
5. In the terms of Grimvall, model ratio of resistivity under the pressure and in the absence of pressure is estimated. It is revealed, for GICs with aluminum chloride very good coincidence between the calculated and the experimental values of resistivity is observed, while for the GICs with bromine calculated and determined experimentally resistivity ratio differ nearly 10 times.

Сопротивление интеркалированных соединений графита с бромом и хлоридом алюминия под давлением

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В статье представлены результаты исследования сопротивления интеркалированных соединений графита акцепторного типа в области температур фазового перехода в слоях интеркалянта. Выявлены особенности фазовых переходов в слоях интеркалянта в интеркалированных соединениях графита под действием давления и температуры. Показано, что сопротивление интеркалированных соединений графита возрастает под давлением, температура фазового перехода в слое интеркалянта сдвигается к более высоким температурам. Оценены параметры электронной структуры интеркалированных соединений графита и их зависимость от давления. Рассчитаны изменения сопротивления интеркалированных соединений графита под давлением.

Ключевые слова: Интеркалированное соединение графита, Удельное сопротивление, Фазовый переход, Слой интеркалянта.

Опір інтеркальованих сполук графіту з бромом та хлоридом алюмінію під тиском

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У роботі представлені результати досліджень опору інтеркальованих сполук графіту акцепторного типу в області температур фазового переходу в шарах інтеркалянту. Виявлені особливості фазових перходів в шарах інтеркалянту в інтеркальованих сполук графіту під дією тиску та температури. Показано, що опір інтеркальованих сполук графіту зростає під тиском, а температура фазового переходу в шарі інтеркалянту зсувається в бік вищих температур. Оцінені параметри електронної структури інтеркальованих сполук графіту та їх залежності від тиску. Розраховані зміни опору інтеркальованих сполук графіту під тиском.

Ключові слова: Інтеркальована сполука графіту, Питомий опір, Фазовий перехід, Шар інтеркалянту.

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