CHARGE CARRIERS ENERGY SPECTRA IN ANISOTROPIC AND BOUNDED STRUCTURES

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In this paper we shall study crystalline structures where translational symmetry of the atom (ion) distribution of the electron (or hole) system is broken by the spattering and due to existence of two boundary surfaces. This is a model of high-temperature superconductors in which the observed symmetry breaking orthogonal to CuO planes was treated as a perturbation. The single-particle fermion wave functions and the possible energies of charge carriers were determined. The competitive existence of the superconductive and normal regions in such sample was shown in agreement with experimental data. The conditions for the formation of superconductive states and the limitations on current density values in the planes parallel to boundary surfaces (in CuO planes) were obtained and discussed.

The answer to the question of the oxide ceramics superconductivity mechanism must be undoubtedly sought in the phonon subsystem, in the elementary charges subsystem as well as in the interaction of these subsystems. With regard to the very anisotropic structure of the superconductive ceramics [1-3], we have attempted to construct a theoretical model conveying the broken translational symmetry of atoms (or molecules) arrangement along one direction in the crystal lattice, the difference of masses of these molecules and the presence of two boundary planes along this direction [4].

The phonon system is drawn out in this model [5]. We have determined the phonon states and their energy spectra and we have shown that, due to the broken crystal symmetry (actually because of deformed and tiny granular structure), the phonons of optical type owning the energy gap are present here. The next task that we have attempted to solve is to determine and analyze the spectra of free charge carriers (electrons or holes), Landau criterion, the probabilities of states and entropy within the same model. The preliminary results are already presented [6-8].

In order to obtain Hamiltonian of the charge carriers in the structure with broken translational symmetry, it is the most suitable to start with the standard Hamiltonian of electron system in an ideal infinite structure:

$$H_{ad} = \sum_k \frac{\hbar^2 k^2}{2m^*} C_k^+ C_k,$$  \hspace{1cm} (1)

where $m^*$ is electron effective mass, while $C_k^+$ and $C_k$ are Fermi creation and annihilation operators of electrons with momentum $\hbar k$ and energy $\hbar^2 k^2/(2m^*)^{-1}$. If we go over to the
configuration space using the transformations:

$$C_k = \frac{1}{\sqrt{N}} \sum_a C_{ak} e^{-i k \cdot \vec{r}_a} ; \quad C_k^+ = \frac{1}{\sqrt{N}} \sum_a C_{ak}^+ e^{i k \cdot \vec{r}_a} ,$$  \hspace{1cm} (2)

where \( N \) is the number of molecules in the considered structure, we get:

$$H = \sum_a \Lambda C_{ak}^+ C_k - \sum_{a,m} W_{am} C_{ak}^+ C_{km} ,$$  \hspace{1cm} (3)

where:

$$\Lambda = N^{-1} \sum_k \frac{\hbar^2 k^2}{2m^*} ; \quad W_{am} = -N^{-1} \sum_k \frac{\hbar^2 k^2}{2m^*} e^{i k (\vec{r}_a - \vec{r}_m)} .$$

Due to the canonicity of the transformation (2), the operators \( C_{ak}^+ \) and \( C_k^+ \) are also Fermi operators.

Let us recall the most important assumptions of our model: we consider the tetragonal i.e. generalized cubic structure with very high anisotropy along the \( z \) axis. That means that the lattice constant in this direction \( a_z \) is a few times larger than the lattice constant \( a_x, a_y \) in the directions \( x \) and \( y \). The translational symmetry is fully conserved in the \( XY \) planes, while the symmetry of the mass arrangement along the \( z \) direction is broken (during the doping of the ceramic structure by the introducing of foreign atoms, the sputtered atoms locate along this direction because it is energetically most convenient). We also assume here that the structure under consideration is a film (not necessarily thin!). It means that the components of lattice vector \( \vec{r} \equiv (n_x, n_y, n_z) \) vary in the following way:

$$n_r \in \left( -\frac{N_z}{2}, +\frac{N_z}{2} \right) ; \quad r = (x, y) ; \quad n_z \in [0, N_z] .$$  \hspace{1cm} (4)

The numbers of atoms \( N_x \) and \( N_y \) along the directions \( x \) and \( y \), respectively, may be indefinitely high, since we have the translational symmetry along these directions. The number of atoms along \( z \) direction \( (N_z) \) is limited. The above described model, i.e. the highly anisotropic matrix along the \( z \) direction, necessarily doped with foreign atoms, can be used for getting some qualitative conclusions about the superconductive ceramics behaviour. It is known [1] that the ceramic oxides are anisotropic along one privileged direction and that the superconductive state is realized by doping. But the real structure of the ceramic oxides - perovskites is approximated by the tetragonal structure. It is also assumed in the model that the spattering is symmetric on the both of boundary planes: \( n_x = 0 \) and \( n_x = N_x \) and between the layers \( n_x = 0 \) and \( n_x = 1 \) (as well as between the layers \( n_x = N_x - 1 \) and \( n_x = N_x \)). The foreign particles are placed, in such a way that the structure of the doped matrix is unchanged near the middle of the film.

In above described model the nearest neighbours approximation was used as well as the continual approximation:

$$f_n \pm 1 \approx f(z) \pm \frac{\partial f}{\partial z} + \frac{a}{z} \frac{\partial^2 f}{\partial z^2} .$$

The system was analyzed throughout the expansion coefficients \( \Lambda \) (of these one-particle function has to be normal

$$\frac{L}{2\alpha} \sqrt{\Phi \left( E - E_i^0 \right)} \Psi,$$

where \( L \) is film thickness, \( \Phi = h n_q (n_0 - Q) \)

$$Q \equiv Q_{ab} = W_{ab} .$$

Consequently, electron energies are described by:

$$E_{1,2} = 4Q + 2b^2 (2\mu + 1) .$$

where \( b = a_z/L \).

It should be pointed out that the long range doping. This energy, after some approximation

$$E_1 = E_{2} + 4b^2 (2\mu + 1) .$$

These elementary excitations are, presumably, superconductivity.

The particular features of high-temperature superconductivity are their granular structure and a weak isotropic effect and Cooper pairs in the conventional superconductor's critical temperature. For that reason [3,9-11], we have proposed the model of cubic structure in which interatomic distance is larger than along other two directions. These atoms locate themselves just along the \( z \) axis. The analysis of phonon spectrum is optical type only in the spectrum (for high energies) it is necessary that the energy

The analysis of electron spectrum in respect to the planes \( n_x = 0 \) and \( n_x = N_x \) boundaries along \( z \) axes, we have two types of excitation: Lower value of energy is related to moving on the sputtering. This term defines value of energy in the spectrum of
The system was analyzed throughout one-particle wave function. It turned out that the expansion coefficients \( A \) (of these states) satisfy Hermite-Weber equation [6]. Since one-particle function has to be normalized the necessary condition arises:

\[
\frac{L}{2a_s} \sqrt{\Phi \left( E - E_z^{(0)} \right)} W_z = 2\mu + 1; \quad \mu = 0, 1, 2, \ldots,
\]

where \( L \) is film thickness, \( \Phi = \hbar n_0 (n_0 + 1)^{-1} \) and:

\[
Q \equiv Q_{\alpha\beta\gamma} = W_z \sin^2 \left( \frac{a_x k_x}{2} \right) + W_y \sin^2 \left( \frac{a_y k_y}{2} \right) + \epsilon_{6}^{(n+1)}.
\]

Consequently, electron energies are discrete ones. Two energy levels appear and they are given by:

\[
E_{1,2} = 4Q + 2b^2(2\mu + 1)^2 \Phi W_z \left\{ 1 \pm \left. \left[ 1 - \frac{2}{(2\mu + 1)^2 b^2 \Phi} \right]^{1/2} \right. \right\},
\]

where \( b = \overline{a}_c / L \).

It should be pointed out that the lower energy of this level is the consequence of the doping. This energy, after some approximation is given by:

\[
E_1 = E_z^{(0)} + 4b^2(2\mu + 1)^2 \Phi W_z - \frac{W_z}{2(2\mu + 1)^2 b^2 \Phi}.
\]

These elementary excitations are, probably, responsible for high critical temperature of superconductivity.

The particular features of high-temperature superconductors on the basis of oxide ceramics are their granular structure and the anisotropy of properties. The existence of the weak isotropic effect and Cooper pairs of charge carriers is experimentally verified, similar as in the conventional superconductors, but BCS model was not able to explain high critical temperature. For that reason and on the basis of established experimental results [3,9-11], we have proposed the model of ceramic structure as tetragonal i.e. generalized cubic structure in which interatomic distances along one direction are few times bigger than along other two directions. It is, energetically, most convenient if the sputtered atoms locate themselves just along this direction.

The analysis of phonon spectrum in our model yields that we have phonon branches of optical type only in the spectrum (there exists energy gap). It means that for phonon excitation it is necessary that the energy (heat) is bigger than the energy gap. The analysis of electron spectrum in these symmetrical deformed structures (with respect to the planes \( n_x = 0 \) and \( n_y = N_x \)) yields that, as a consequence of existence of the boundaries along \( z \) axes, we have two energy branches in the spectrum of charge carriers. Lower value of energy is related to more populated states and contains the term depending on the sputtering. This term decreases with increasing of the film thickness. Higher value of energy in the spectrum of charge carriers is not particularly analyzed because
these levels are low populated.

In addition to this, in the framework of model under consideration we have determined the orthonormalized single-particle state functions of this system, entropy and the probabilities of possible states. The theoretical investigation in the framework of presented model is not finished. It is necessary to form Hamiltonian of the interaction between charge carriers and phonons and separate from it the essential part only, which describes the formation of Cooper pairs. Only after this the thermodynamical analysis of the complete system follows.

References

1. J.G. Bednorz and K.A. Müller: Perovskite-Type Oxides - the New Approach to High-
   and T.M. Shaw, The Structure of $Y_1Ba_2Cu_3O_7-\delta$ and its Derivatives, K.C. Hass,
   Electronic Structure of Copper-Oxide Superconductors, in Solid State Physics -
   Advances in Research and Applications, Eds. H. Ehrenreich and D. Turnbull, Vol. 42
6. J.P. Šetrajčić, B.S. Tošić and D.Lj. Mirjanić, Spectra and States of Charge Carriers
   in Anisotropic and Bounded Structures, 10th General Conference of the European
   Physical Society, Sevilla 1996.
7. J.P. Šetrajčić, S.M. Stojković, B. Abramović and S. Lazarev, Bal. Phys. Lett. 5/2, 414
   (1997).
   Timişoara (Mat. Fiz.) 43, 121 (1998).

Some properties of the ionomeric

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Summary

Polyurethane catenomers based
and N-methyldecanalaminolamine quaternari
reaction between the tropylium ion
sodiumpropylsulfonate, azaaromatic dyes
azo dye (methyl orange) in the same properties
both in polymer solution and

Introduction

Polymers with azoaromatic groups and a number of papers have been published
great versatility of polyurethanes and materials carrying azoaromatic chromophores
taking into account the development of biological systems [1-3]. Despite a few examples in literature describing
introduced in their main chains [4].

Our program concerning the azoaromatic functionality [5-7], has
ionomeric architecture, which combine from co-existence of minority of ion
properties to form aqueous dispersions
them suitable for a myriad of applications
this direction, polyetherurethane co
dibenzylmidozoycane and N-methyl
 groups were synthesized and character
radiation was evidenced by electronic
some sensitive and thermal probe
comparatively with non-ionic polyurethanes

Experimental Part

Synthesis of 1,4-polyazobenzene
0.01 mol of sodium/p-hydroxyazo
0.011 mol of p-propylalcohol in the
under reduced pressure, the resulting

40 v/v).