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The Forming Factors of High Values of Superconducting Transition Temperature T_c in 3*d*-Transition Metal Compounds

II. Empirical and Theoretical Equipments for Receiving the Values of Superconducting Transition Temperature T_c

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Abstract

The review of empirical and theoretical studies of the superconducting transition temperature is presented. It is shown that correlation between the parameters of chemical bonds and the value of the superconducting transition temperature is realized.

Keywords: Superconducting transition temperature, Electronegativity, Chemical hardness

From the results of review published in [1] we conclude that the large part of modern investigations deals with problems of building of microscopic theory of superconductivity. According to [2] empirical investigations of superconductors show that in materials at transition to superconducting state near the temperature T_c the superconducting gap E_g appears. It is possible to expect, that serial numbers of elements in Periodic system and a degree of elasticity of of interatomic interactions can influence on ratio a = $E_g / k_B T_c$.

In work [2] four basic approaches to description the effect of superconductivity are submitted: 1) thermodynamical; 2) based on London equation; 3) theory of Bardeen-Cooper-Schrieffer (BCSh) [3]; 4) phenomenological theory of superconductors of first and second type introduced by Ginzburg, Landau, Abrikosov and Gor'kov [4].

According to our opinion in above mentioned list of basic approaches must be added quantum-mechanical relaxational one which uses the definition of electronegativity.

First the definition of electronegativity was submitted by L. Poling at 1932 and given, for example, in [5].

The next main improvements of that definitions included: 1) transition according with ideas of Mulliken from electronegativity of atom or ion up to the electronegativity of the valence orbital; 2) establishing in 60 -th years last century by a group of authors [6] the empirical rule that for free atom the energy of one shell is the function of number occupation by electrons q and in total may be approximated by power series $E(q) = E(0) + \alpha q + \beta q^2 + \gamma q^3 + ...$, where α, β, γ – empirical parameters, $E(0)$ – energy of ionized core; 3) assumption of that energy $E(q)$ can be considered as continuous function from q within interval $0 < q < 2$. Then within under linear approximation with respect to charge q (i.e. assuming that γ=0) electronegativity it is possible to define as a derivative of energy of atoms on the electronic occupation number of valence orbital or as potential which acts on partially filled valence orbital: $\chi(q) = dE(q)/dq = \alpha + 2\beta q$. Slater in [7] within X_α-method of self consistent field substantiated the expansion of energy of atom as function of number occupation q. In [7] Slater specially pointed, that fundamental equations of X_α-method unlike classic Hartree-Fock method has not restrictions bonded with requirements of integer values of q. This is the one of the reasons of that X_α method more correctly define the properties of molecules or crystals in comparing with the Hartree-Fock method, because atomic systems with semi integer values of spins obey Fermi statistic for which the fractional occupation numbers of energetic levels are more typical; 4) a different approach for justification of continuity of expanding $E(q)$ give the density functional theory. Within this formalism by Parr and others [8] were showed that electronegativity χ can be considered as taken with opposite sign the chemical potential μ of electrons in N-electronic system $\mu = \left[\frac{\partial E(\rho)}{\partial \rho}\right]_V = \left(\frac{\partial E}{\partial N}\right)_V = -\chi$. In this case χ coincides with orbital electro-negativity. Parr and Pearson in [9] substantiate the hypothesis about that the

second derivative of energy on number of electrons is the important chemical characteristic which was named as the chemical hardness η: $\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_V$. In other form: $2\eta = \left(\frac{\partial \mu}{\partial N}\right)_V = -\left(\frac{\partial \chi}{\partial N}\right)_V$. The last expression shows that chemical hardness η is the "resistivity" of chemical potential of elements (or electronegativity) with changing number of electrons. Finally for function of electronegativity it is possible to write the following expression $\chi = \left(\frac{\partial E}{\partial N}\right) = \chi^0 + 2\eta^0 q$, where χ^0 - electronegativity of neutral atom, *q*- the number (usually fractional) of electrons, taken part in process of transition (ionization).

Authors of [10] considered the possible performance criteria of superconducting realization based on the effective charges Q_{eff}, electronegativity χ, partial electronegativities f_{k}, average electronegativities of elements χ_{aver}, difference of electronegativities $\Delta\chi = \chi_A - \chi_B$. Within article [11] are introduced the approach which connect of electronegativities of metal and oxygen atoms with type of chemical bonding, realized between the atoms: ionic, covalence and metallic; it was showed that electronegativity of arbitrary group of atoms may be evaluated using the electronegativities of atoms of separate elements. Results of [12] tell us that electronegativities which calculated by Mulliken method can be used for the analysis of dependence of temperature superconducting transition T_{c} from type of chemical bonding. Authors of article [13] submitted the results of application of method based on the using of different electronegativities for atoms of f-elements and allowed adequately carry out the theoretical description of electronic structure of metal sublattice in superconductor.

In conclude, there is the necessity in clear definition of physical meaning of value of electronegativity; introducing physical unit for electronegativity; working-out the based on electronegativity the quantitative characteristic which can be used as test for condition of realization of superconductivity effect; definition the nature of numerical coefficient *a* from expression $E_g \sim a \times k_B T_c$ which connect values of superconducting gap E_g and superconducting transition temperature T_c.

In the next report III we assume to consider the features of superconducting transition basing on introduced by us quantum mechanical relaxational model of superconducting transition.

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