Numerical Approach in Superconductivity

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Abstract. The dependence of the critical temperature of high temperature superconductors of various families on their composition and structure is proposed. A clear dependence of the critical temperature of high temperature superconductors on the sequence number of the constituent elements, their valency, and the structure of the crystal lattice is revealed.

Keywords: High-temperature superconductivity; critical temperature.

1 Introduction

Recent results in high-temperature superconductivity have led to great interest of the scientific community in the search for a theoretical explanation of the mechanism of the appearance of a superconducting state at temperatures close to room temperature. Nevertheless, many theoretical questions remain unresolved, while the experiment came close to room temperature at high pressures, and half way to room temperature at normal pressure.

In this paper, an attempt is made to establish a relationship between the temperature of the superconducting transition T_c various families of high-temperature superconductors on the composition and structure of the material of the superconductor. To do this, a numerical approach is used, similar to Balmer's work using number theory, which was only once applied to fundamental problems of physics more than a hundred years ago in the description of the spectra of hydrogen radiation [1]. His result was confirmed by Rydberg [2] and explained by Bohr when he created quantum mechanics [3].

2 Method and Results

The essence of the applied method is as follows. Consider a Hg-based cuprates $Hg_mBa_2Ca_{n-1}Cu_nO_{2n+m+2}$ or by another designation $Hg-m2(n-1)n$. Assume that T_c is proportional to the combination of integers, the serial number of the elements of a given cuprates, and their number in the chemical formula of the element. It turned out by the enumeration method that the following combination is in good agreement with the experimental value of T_c:

$$\frac{1}{T_c} = \frac{C_0 \cdot n \cdot m \cdot (m+1)/2}{300 \cdot (2N-3)^2}\left(\frac{1}{m \cdot Hg} + \frac{1}{2 \cdot Ba} + \frac{1}{(n-1) \cdot Ca} + \frac{n}{n \cdot Cu + O^{2n+m+2}}\right), \quad (1)$$

where $C_0 = 147.27\,K^{-1}$ is the fitting constant; n and m are integers from the material designation; designation of an element - its serial number, or nuclear charge, i.e. Hg = 80,

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Composition: $Hg-m2(n-1)n$	experimental T_c, [source]	T_c by the formula (1)	T_c by the formula (2)
$Hg-1201$	$97\,K$ [4]	$95\,K$	$134\,K$
$Hg-1212$	$128\,K$ [4]	$128\,K$	$140\,K$
$Hg-1223$	$135\,K$ [4]	$132\,K$	$152\,K$
$Hg-1234$	$127\,K$ [4]	$120\,K$	$144\,K$
$Hg-1245$	$110\,K$ [4]	$108\,K$	$132\,K$
$Hg-1256$	$107\,K$ [4], $92\,K$ [5]	$97\,K$	$121\,K$
$Hg-1267$	$88\,K$ [4]	$88\,K$	$111\,K$
$Hg-1278$	$< 90\,K$ [4]	$80\,K$	$103\,K$
$Hg-2212$	$44\,K$ [4]	$47\,K$	$48\,K$
$Hg-2223$	$45\,K$ [4]	$51\,K$	$53\,K$
$Hg-2234$	$114\,K$ [4]	$48\,K$	–

Table 1: Table of experimental values of the critical temperature of Hg-based cuprates in comparison with calculated by formulas (1−2).

Ba = 56, Ca = 20, Cu = 29, O = 8; N is the number of elements, not counting Cu-O: for example, N = 2 for Hg-1201 (here two elements are mercury and barium), N = 3 for 1212 (here mercury, barium and calcium), etc.

Table 1 shows the transition temperatures calculated by formula (1) and taken from the literature.

It was further assumed that the crystal lattice remains the same (we do not change all the coefficients in formula (1)), but we introduce mercury atoms in the crystal cell - we increase the coefficient at Hg by one, leaving m unchanged:

$$\frac{1}{T_c} = \frac{C_0 \cdot n \cdot m \cdot (m+1)/2}{300 \cdot (2N-3)^2}\left(\frac{1}{(m+1)\cdot Hg} + \frac{1}{2\cdot Ba} + \frac{1}{(n-1)\cdot Ca} + \frac{n}{n\cdot Cu + O^{2n+m+2}}\right). \quad (2)$$

In table 1, the calculation according to formula (2) is shown in the 4th column for samples (hypothetical) with mercury atoms embedded in the crystal lattice. For a material with m = 1, an increase in T_c is visible. The coincidence of $T_c = 152\,K$ for Hg-1223 calculated according to (2) with the transition temperature of the Hg-1223 sample at a pressure of $P_0 = 150\,kbar$ [6] can be considered is not accidental, assuming that introducing mercury atoms into the crystal cell of Hg-1223, creates mechanical stresses equivalent to those at the specified external pressure P_0.

Considering the position of the nodes of the Hg-1223 crystal lattice to be unchanged when mercury atoms are introduced into it (from one to eight intruding atoms), the value of mechanical stresses in the Hg-1223 crystal cell was estimated. The parameters of the Hg-1223 cell are $a = 3.85\,\mathring{A}$, $c = 15.8\,\mathring{A}$ [7].

The total energy of elastic deformation of the crystal cell [8]:

$$W = 8 \cdot \pi G \cdot r_0 (r_1 - r_0)^2, \quad (3)$$

where $G = 27.6\,GPa$ - the shear modulus is taken for another cuprate $Tl_2Ba_2CaCu_2O_{8+\delta}$ [9], because for Hg-based is not yet found in the literature; $r_0 = 1\,\mathring{A}$ is the radius of the

sphere in the cell where the mercury atom is introduced (taken offhand for a preliminary estimate); $r_1 = 1.55\,\mathring{A}$ is the radius of the mercury atom.

The total energy of elastic deformation of the lattice cell upon the introduction of one mercury atom: $W = 2.1 \cdot 10^{-19}\,J$. When eight mercury atoms are introduced into the cell, i.e. as much as in the nodes of the cell Hg-1223: $W = 16.8 \cdot 10^{-19}\,J$. Then the mechanical stress in the cell in the latter case:

$p = \frac{W}{a \cdot a \cdot c} = \frac{16.8 \cdot 10^{-19}}{a \cdot a \cdot c} = 80\,kbar$, which coincides with P_0 in order of magnitude.

Thus, it has been shown that the incorporation of mercury atoms into the lattice cells of the Hg-1223 sample creates mechanical stresses in the crystal lattice equivalent to those at increased external pressures into which the ordinary Hg-1223 sample is placed.

Further analysis of formula (1) revealed that the combination $300 \cdot 2/C_0$ coincides with the average temperature T_c for $\alpha-$ and $\beta-$modifications of mercury: $T_c^{Hg} = 300 \cdot 2/C_0 = 4.074\,K$ [10], [11]. Then formula (1) can be rewritten in the form:

$$\frac{1}{T_c} = \frac{n \cdot m \cdot (m+1)}{T_c^{Hg} \cdot (2N-3)^2}\left(\frac{1}{m \cdot Hg} + \frac{1}{2 \cdot Ba} + \frac{1}{(n-1) \cdot Ca} + \frac{n}{n \cdot Cu + O^{2n+m+2}}\right), \tag{4}$$

where the superscript at T_c simply denotes the element, and not the value of the element's serial number, as is done in brackets.

Using the same approach as for cuprates and taking into account the last nuance regarding the nature of the constant, a formula is obtained that establishes a relation between the temperature of the superconducting transition and the composition of the material of high-temperature superconductors of the AH_n or AD_n family of hydrides, where $A = S, La, Y, Pr$:

$$\frac{1}{T_c} = \frac{1}{T_c^A \cdot (2N+1)}\left(\frac{1}{A} + \frac{h}{n}\right), \tag{5}$$

where T_c^A is the critical temperature of the Ath element (table 2) and the superscript A is just the designation of the element; in brackets A - serial number (nuclear charge) of the element; n is integer from the material designation; h is an integer or rational number depending on the crystal group of the sample (table 2); N is the number of elements in the substance - everywhere N = 2, because there are always two elements: A and hydrogen, or deuterium.

Table 2 shows the transition temperatures calculated by formula (5) and taken from the literature. The value of h (in table 2) has a certain value for each crystalline group.

In the case of praseodymium, there is no data at ultrahigh pressures of the order of 100 GPa or more. Therefore, it can be expected that Pr will be superconducting with a critical temperature near 2 K at about 100 GPa or more.

As a next step, a formula establishing the relationship between the temperature of the superconducting transition and the composition of the material of high-temperature superconductors of the yttrium-based cuprate family $Y_m Ba_k Cu_n O_p$ was obtained based on previous results:

$$\frac{1}{T_c} = \frac{n_a \cdot (n_a + m) \cdot m(m+1)}{T_c^Y \cdot 2N}\left(\frac{1}{m \cdot Y} + \frac{1}{k \cdot Ba} + \frac{n}{n \cdot Cu + O^p}\right), \tag{6}$$

Composition: AH_n	crystal group	experimental T_c, [source]	T_c by the formula (5)	T_c^A, [source]	h
H_3S	$Im-3m$	203.5 K at 155 GPa [12]	202.1 K	$T_c^S = 16\,K$ at 160 GPa [17]	1
D_2S	$Im-3m$	150 K at 155 GPa [12]	142 K	$T_c^S = 16\,K$ at 160 GPa [17]	1
LaH_{10}	$Fm\bar{3}m$	260 K at 200 GPa [13]	253 K	$T_c^{La} = 5.95\,K$ at ambient pressure [18]	1
LaD_{11}	$P4/mm$	140 K at 142 GPa [14]	149 K	$T_c^{La} = 5.95\,K$ at ambient pressure [18]	2
YH_6	$Im-3m$	227 K at 237 GPa [15]	241 K	$T_c^Y = 9.27\,K$ at 31 GPa [19]	1
YH_9	$P6_3/mmc$	243 K at 201 GPa [15]	241 K	$T_c^Y = 9.27\,K$ at 31 GPa [19]	6/4
PrH_9	$P6_3/mmc$	55 K at >110 GPa [16]	54.4 K	$T_c^{Pr} = 2\,K$	6/4
PrH_9	$F\bar{4}3m$	69 K at 120 GPa [16]	61 K	$T_c^{Pr} = 2\,K$	4/3

Table 2: Table of experimental values of the critical temperature of hydrides in comparison with calculated by formulas (5).

Composition: $Y_mBa_kCu_nO_p$	experimental T_c, [source]	T_c by the formula (6)
$YBa_2Cu_3O_7$	92 K [20]	89 K
$YBa_2Cu_4O_8$	80 K [20]	89 K
$Y_2Ba_4Cu_7O_{14}$	40 K [20]	45 K

Table 3: Table of experimental values of the critical temperature of Y-based cuprates in comparison with calculated by formulas (6).

where $T_c^Y = 9.27\,K$ is the critical temperature for yttrium at 31 GPa [19]; m, k, n and p are integers from the material designation; designation of an element - its serial number, or nuclear charge, i.e. Y = 39, Ba = 56, Cu = 29, O = 8; N is the number of elements, not counting Cu-O: i.e. N = 2; n_a is the number of $Cu-O$ planes in the crystal cell [20] (always equal to 2).

Table 3 shows the transition temperatures calculated by formula (6) and taken from the literature.

In the derivation of (6), another values was also used $T_c^Y = 7.9\,K$ at 26 GPa [19] and $T_c^Y = 1.5-2.7\,K$ at 12-16 GPa [21], but the best formulas obtained with a slightly different combination of numbers in front of the brackets gave much worse agreement with the experiment. This suggests that the mechanical stresses in the crystal cell of the Y-based cuprates are close to 30 GPa, at least in the vicinity of the Y atom.

3 Conclusion

Using numerical approach, formulas are derived that relate the temperature of the superconducting transition to the composition and structure of the material for various families of superconductors. A prediction is made about a method for increasing T_c for Hg-based cuprates by implanting Hg atoms in the cuprate crystal lattice, which will create mechanical stresses in the lattice equivalent to those with increased external pressure.

It is not surprising that T_c would have a systematic dependence on integers, since the consensus view of superconductivity, regardless of physical instantiation, is that of Cooper pairs, formed via the exchange of a boson. The pairing will depend in a systematic way on the coupling to this boson, the characteristic energy of this boson, and the density of states. All of these quantities reflect the constituent elements in the superconducting compound and, as such, are subject to the systematic variation of elemental properties embedded in the periodic table.

The method was applied to the recently discovered hydrides and this algorithm gives agreement with the observed transition temperatures. It is necessary to test this method to other superconductors at high pressures in order to reveal its validity and the laws behind it. Because the main goal of the study is to find a general law and predict material with the desired T_c at any pressure.

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