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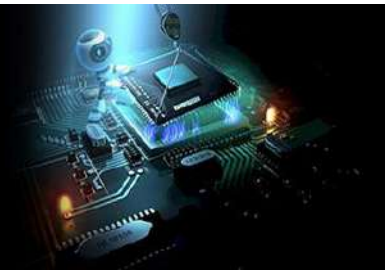

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Mathematical optimization and approximation methods for primary molecular effect model in high temperature superconductors TL group [TC > 0°]

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Abstract
Optimization-Modelling Molecular Effect methods for one HTSC group were approached/determined based on previous studies. Namely, Inverse Least Squares (ILS), 2D Numerical/Graphical Optimization in primary Molecular Effect model are presented. This contribution results deals with the Molecular Effect Model ILS Numerical/2D Graphical modelling for High Temperature Superconductors HTSCs group of [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] whose TC > 0° C exclusively. This HTSCs class, among others, constitutes a recent materials innovation in HTSCs with both TC > 0° C and TC < 0° C material compounds. It shows important recent/prospective electronics physics applications. For results with these optimization/simulations, classical ILS, 2D Interior Optimization, and 2D Graphical Optimization techniques are applied. Numerical-Imaging solutions comprise Tikhonov Regularization algorithms and mathematical modelling-methods for this HTSCs group. Primarily, results prove a 2D sinusoidal analytic geometry model curve. Findings for this Molecular Effect ILS optimization show acceptable theoretical Numerical, 2D Graphical Optimization outcomes with low residuals. Results comprise two strands, the modelling for TC Molecular Effect, and the ILS software/imaging methods. HTCS Electronics Physics applications emerge from numerical and graphical results.

Keywords: Interior Optimization (IO) Methods, Graphical Optimization, Systems of Nonlinear Equations, Tikhonov Regularization (TR), Critical temperature [Tc], Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory, [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Molecular HTSC Group, Molecular Mass (MO)

Introduction
Following a series of contributions in Superconductors Modelling Optimization [1, 4-6], a new HTSCs class is studied in this article. The subject of the research is the HTSCs group [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] whose TC > 0° centigrades exclusively. This HTSCs class, among others, constitutes a recent materials innovation in HTSCs with TC ϵ [230 °K, 80 °C] approximately for their material compounds [3-5, 12-15, 32-34, 37]. That is a significant thermodynamical-materials difference compared to other HTSCs classes.
The classical BCS theory is based on a chain of interactive physical-chemical phenomena, supported by a number of physical-chemical equations with extensive mathematical basis. In plain language, namely, [thermodynamical effect of material-cooling summed to electrical J → electrons-subsequent lattice deformation with electrical-resistance decrease → phonons production → high acceleration of current of electrons]. However, theoretical superconducting background is rather complicated as it involves physics and chemistry matter models, quantum mechanics theory, and extensive algorithms with variations [3-5, 12-15, 32-34, 37]. HTSCs belong to so-called Type 2 Superconductors, the most recent/innovative group in continuous improvements/evolution whose probably further industrial applications have got going be discovered. Studies on matter structure, currently try to explain the Type 2 metallic compounds and alloys superconducting effect sorting rather difficult theoretical and experimental hurdles. Type 2 superconductors show different properties in superconducting state transition phenomena compared to Type 1 ones [3-5, 12-15, 32-34, 37].
Isotope Effect constitutes a primary milestone when superconducting theory began to find experimental confirmations. Isotope Effect algorithm upholds that differences in atomic mass of a chemical element determines the variable critical transition temperature of a superconductor.

In this line, Molecular Effect hypothesis is based on a similar criterion [Casesnoves, 2020] [1-5]. That is, provided a HTSCs class has a very similar nano-molecular-atomic structure, the variations in TC magnitude within the group could be linked to valences, type of isotopes and proportions in the material mixture. For instance, a mixture of the same compound with several isotopes forming the same molecules.

The presented Molecular Effect model is at hypothesis stage [Casesnoves, 2020, 3-5], since flux-lattice vortices concepts and inter-related physical-chemical equations, among others, are not set yet if they would be necessary.

A previous study showed primary optimization for other class of HTSCs with TC > 0° centigrade [1]. Generally, [1-6, 14-16, 26-29], the classical HTSCs are those ones whose Tc is approximately higher than 80 K—exactly 77 K [3-5, 12-15].

In BCS classical superconductors theory, the Isotope Effect model [1-6, 14-16, 26-29] for uni-element superconductors equation reads,

$$[M_i]^{\alpha} T_C - K \cong 0; \quad \text{for } i = 1,....n; \tag{1}$$

Where K and α are numerical-experimental constants, M Atomic Element Mass (AMU) of an element with (n) isotopes, TC is critical temperature (usually Kelvin); (i) is the corresponding isotope for the element.

In this contribution, the Molecular Effect Model 2D Graphical/Numerical-Algorithms model for HTSCs [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] class are presented. However, the selected compounds for optimization are constrained to those whose TC > 0°.

The Isotope Effect Model, Equation (1), is a simple algorithm based on element-atomic mass of a Type 1 superconductor-element isotope and the Critical Temperature Tc. That is, two main parameters [M, TC], and two constants [K, α] to be determined experimental-numerically. That model has proven be acceptable with some inaccuracies [3-5, 12-15] along the superconducting investigations.

The [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] chemical group whose molecular composition/formulation diverge in proportion of valences/elements [1-9, 12-15] is numerically/graphically optimized with ILS polynomial model [1].

In summary, the article shows a 2D Numerical-Graphical optimization study for the primary hypothesis of Molecular Effect model set on [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs class. Programming-algorithms are implemented with Matlab imaging-processing software and 2D Graphical model plots are also developed with this system. The software constitutes an evolution based on previous research [1, 4-6]. 2D numerical/graphical solutions show low errors and residuals. The model shapes results fit approximately sinusoid curves.

Mathematical Algorithms and Computational Methods

The numerical experimental data for setting the Molecular Effect model for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSC group is shown in Table 1. The differences among the 13 group compounds are given by a number of elements. Tl, Ba, Cu and O, always form molecule part, instead, Sn, Mn, Ti, Si, Pb, and Mg, are complementary in specific compounds within this HTSCs class. Valences are not always discrete figures, and are set without subscript format for clarity. In this HTSCs class, exclusively those compounds whose TC > 0° are selected for the model optimization.

The computational method is similar to [1, 4-6], but in this study the software loops, patterns, and imaging processing tools for 2D Graphical and statistical programming were improved according to this HTSCs class characteristics. Algorithm is based on Tikhonov Regularization Theory [7, 13, 31] and previous contributions.

Numerical Experimental Data

Table 1 presents Numerical Experimental Data for modelling. [3-5, 12-15, 32-34, 37]. There are differences among the respective compounds TC and element-compositions. However, the differences among the Molecular Weights are not significative.

Numerical optimization data [T1-Sn-Pb-Ba-SiMn-Mg-Cu-O] CLASS [HT-Superconductors, [Tc> 0°] Molecular effect hypothesis]	
Formulation	**Molecular Weight (UAM) / Approximate Tc (Centigrade)**
TI7Sn2Ba2MnCu10O20	2.9531e+03 177
TI7Sn2Ba2TiCu10O20	2.9461e+03 1 65
T16Sn2Ba2TiCu9O18	2 6462e+03 / 56
TI7Sn2Ba2SiCu10O20	29263e+03 / 53
T16Ba4SiCu9O18	2.6636e+03 / 48
T15Ba4SiCu8O16	2.4479e+03 / 44
(TI5Sn2)Ba2SiCu8O16	23264e+03 / 42
(T15Pb2)Ba2SiCu8O16	23034e+03 / 38
(T15Pb2)Ba2SI2.5Cu8.5O17	25933e+03 / 35
(T15Pb2)Ba2Mg2.5Cu8.5O17	25839e+03 / 30
(T15Pb2)Ba2Mg2Cu9O18	16195e403 / 28
(T15Pb2)Ba2MgCul0O20	2.6907e+03 / 18
(T14Pb)Ba2MgCu8O13	2.0401e+03 / 3

Table 1.-The development of optimization of parameters for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] class implemented in this study [1, 4-6, 14-16]. Note the differences among the group compounds. Tl, Ba, Cu and O, always form molecule part, but for instance Pb, Mn, Mg, and Si are present exclusively in specific compounds within this HTSC class.

Computational-Software Algorithms

For this Molecular Model optimization, the algorithm with constraints for parameters is shown in Equation (2).

Tikhonov functional method is applied as [1]. Therefore, algorithms set for ILS Molecular Effect, with a polynomial p(MO) read,

$$\begin{aligned}&\text{minimize Tikhonov functional } J(\alpha),\\&\text{with } \alpha 1=0 \text{ and } L_2 \text{ Norm},\\&J_{\alpha}(u)_{uex}=\left\|Au-p(MO)\right\|_2^2+[\alpha 1]\,J(u);\\&\text{Hence minimize},\\&\left\|T_{Ci}-p(MO_i)\right\|_2^2 \quad ,\\&\text{for } i=1,\ldots..n\\&\text{subject to} \quad ,\\&a\le MO_i\le a_1\,;\\&b\le T_{Ci}\le b_1\,;\end{aligned} \tag{2}$$

Where MO_i is the molecular weight of the HTSC selected (i) within a HTSC group with (i) elements, and [a-b] are constraints intervals. T_{Ci} is critical temperature (Centigrades) for every (i) member of HTSCs group. The figure α1 is a constant specific Tikhonov Regularization Parameter, to be appropriately selected. The constraints [a-b] are applied for 2D modelling optimization. This OF was selected with ILS programming in Matlab.

The selected group of HTSCs constitutes a modern HTSCs materials whose $T_C > 0°$ centigrades, with prospective applications [1-6, 14-16, 26-29]. Table 1 shows a narrow T_C differences interval, namely, approximately T_C-Group ϵ [120, 190] centigrades.

Numerical and Graphical Results

Molecular Effect modelling results are 2D Graphical, Figures 1,2, and Numerical, Tables 2,3, with explicit model equations. Matlab Graphical results for 3-degree and 5-degree ILS polynomial model are shown in Figures 1,2. Both 3 and 5-degree show a sinusoid curve-shape for model. Graphical errors can be considered acceptable/low. Results for ILS equations are detailed in Tables 2,3, with approximations and errors.

ILS 3-Degree Graphical Optimization Model Results

Figure 1 shows sinusoid-shaped model curve for ILS 3-degree Molecular effect model in [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. A difference in shape compared to parabolic model-curves obtained in previous studies with different HTSCs class [1, 4-6].

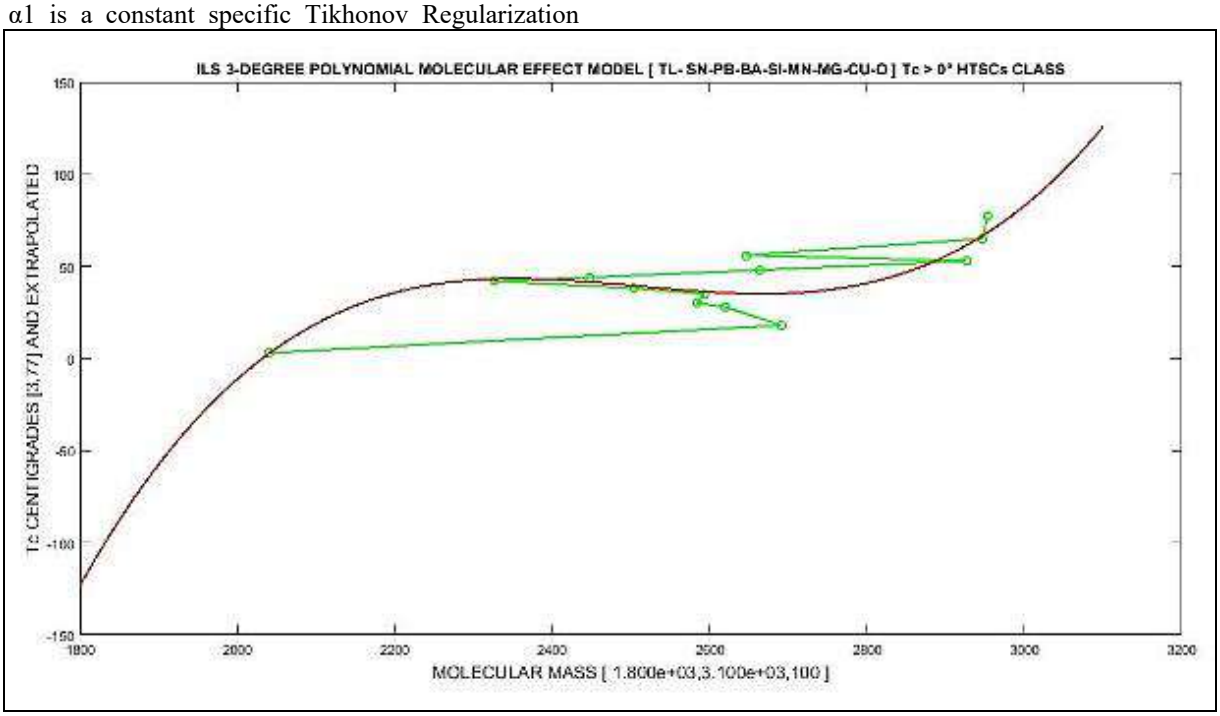

Fig 1: First attempt with 3-degree ILS polynomial optimization of Molecular Effect Model for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. Matlab Extrapolated modelled curve (red) and experimental data (green). The model results to resemble a sinusoid equation, approximately. Since this HTSCs class has a number of compounds with $T_C < 0°$, the model confirms that trend.

ILS 5-Degree Graphical Optimization Model Results

Figure 1 with a 5-degree ILS polynomial model validates sinusoid-shaped model curve for ILS 3-degree Molecular effect model in [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group got at Figure 1. A clear difference in shape compared to parabolic model-curves obtained in previous studies with different HTSCs class [1, 4-6].

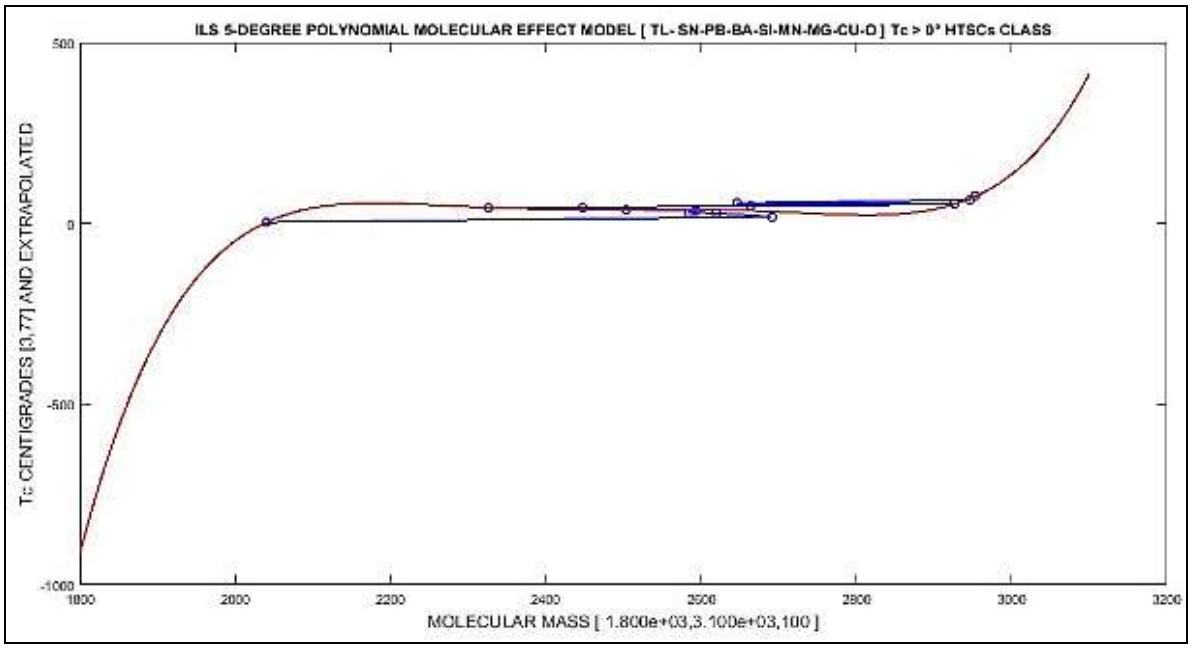

Fig 2: The 5-degree ILS polynomial optimization of Molecular Effect Model for this HTSCs group. It confirms the 3-degree ILS polynomial model analytic geometry shape. Extrapolated modelled curve (red) and experimental data (blue). The model results be almost linear at intermediate values and becomes sinusoid for significant absolute-values increments in $T_C < 0°$ and $T_C > 0°$ [1, 12-15, 32-34, 37].

ILS Model Equations

Tables 2,3 show 3 and 5 ILS model equations without/with approximations, discarding very low polynomial coefficients if numerically necessary.

Table 2: First 3-degree ILS polynomial optimization of Molecular Effect Model Equation. Approximations were not numerically possible since there are not coefficients very high with negative powers.

ILS MOLECULAR EFFECT MODEL (3-DEGREE) WITHOUT APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
8.2906e+003	CONSTANT
10.0383e+000	X
-4.0163e-003	X^2
533.5328e-009	X^3
RESIDUAL = 5.8316e+000	
MODEL EQUATION	
$Tc = [\ 8.2906e+003\ ] + \ldots$ $\ldots + [\ 10.0383e+000\ ]\ MO + \ldots$ $\ldots + [\ -4.0163e-003\ ]\ MO^2 + \ldots$ $\ldots + [\ 533.5328e-009\ ]\ MO^3$	

Table 3: First 3-degree ILS polynomial optimization of Molecular Effect Model Equation. In this case, approximations were numerically possible since there are coefficients very high with negative powers.

ILS MOLECULAR EFFECT MODEL (5-DEGREE) WITH APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
-829.6301e+003	CONSTANT
1.6793e+003	X
-1.3557e+000	X^2
545.7033e-006	X^3
-109.5228e-009	X^4
≈ 0	X^5 [not significant]
RESIDUAL = 5.6351	
MODEL EQUATION	
Tc = [-829.6301e+003] +... ... + [1.6793e+003] MO + ... +[-1.3557e+000] MO^2 +... ...+ [545.7033e-006] MO^3 +... ...+ [-109.5228e-009] MO^4	

Discussion and Conclusions

The objective of this study was to get a graphical/numerical model for Molecular Effect Model in [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs class subject to $T_C > 0°$ C. Recently, this HTSCs materials are in current research/evolution because of their electronical-thermodynamical properties. In this HTSCs group, Molecular Effect model was 2D graphically and numerically determined.

Results have two branches, Graphical and Numerical ones for this HTSC group Molecular Effect Algorithms. Primarily, can be considered acceptable with low residuals. In contrast with previous research for other groups of HTSCs materials [1, 4-6], the model shows a sinusoid clear analytic geometry shape. It does not depend on ILS polynomial-model degree selected. Equations/ Approximations for 3 and 5 degree ILS polynomial methods have been obtained and approached.

Engineering-Software and programming-patterns are based on previous contributions [1-9, 17-25]. Specific modifications were applied for the proper characteristics of the HTSCs materials class to show sharply this new sinusoid analytic geometry.

In brief, 2D ILS polynomial-modelling Graphical Optimization methods for HTSCs group [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] materials have primarily determined. Applications in Electronics Physics turn up from the study Numerical/Graphical findings.

Scientific Ethics Standards

The study comprises a totally new class of HTSCs materials. Molecular Effect model was created by author in 2020-1. Equations set are algorithms previously used for different materials class models. 2D/3D Graphical Optimization Methods were created by Dr Francisco Casesnoves in 3rd November 2016, and Interior Optimization Methods in 2019. 2D/3D/4D Graphical and Interior Optimization Methods were created by Dr Casesnoves in 2020. This article has previous papers information, from [1, 4-6], whose inclusion is essential to make the contribution understandable. The 2D Graphical Optimization in Matlab constitutes a software engineering improvement from previous contributions [1, 3-9]. The 2D/3D/4D Interior Optimization method is original from the author (August 2020-1). This study was carried out, and their contents are done according to the International Scientific Community and European Union Technology and Science Ethics [38-41]. References [40, 41] and [38, 39]: 'European Textbook on Ethics in Research'. European Commission, Directorate-General for Research. Unit L3. Governance and Ethics. European Research Area. Science and Society. EUR 24452 EN [37-40]. And based on 'The European Code of Conduct for Research Integrity'. Revised Edition. ALLEA. 2017. This research was completely done by the author, the computational-software, calculations, images, mathematical propositions and statements, reference citations, and text is original for the author. When a mathematical statement, algorithm, proposition or theorem is presented, demonstration is always included. If any results inconsistency is found after publication, it is clarified in subsequent contributions. The article is exclusively scientific, without any commercial, institutional, academic, religious, religious-similar, non-scientific theories, personal opinions, political ideas, or economical influences. When anything is taken from a source, it is adequately recognized. Ideas and some text expressions/sentences from previous publications were emphasized due to a clarification aim [38-41].

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