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Mathematical 3D Graphical Optimization and Approximation Methods for Primary Molecular Effect Model in High Temperature Superconductors [Sn-Sb-Te-Ba-Mn-Cu-O] Group

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Abstract

In previous research, Molecular Effect Model (MEM) with Inverse Least Squares (ILS) 2D Numerical/Graphical Optimization methods for [Sn-Sb-Te-Ba-Mn-Cu-O] High Temperature Superconductors (HTSC) class were presented. This HTSCs Critical Temperature group [Sn-Sb-Te-Ba-Mn-Cu-O] has the characteristic $T_C > 0°$ for all its compounds. Results in this contribution show three main parts. Namely, MEM equations/algorithms, MEM equations approximations, and 2D/3D MEM Graphical Optimization. Solutions involve Tikhonov Regularization algorithms and mathematical methods for this HTSCs group. Mathematical-programming outcomes for optimization this Type II HTSCs are demonstrated with ILS polynomial data in Matlab and GNU-Octave. Rulings present acceptable Numerical and 2D/3D Graphical Optimization solutions. Results show software-programming improvements in accuracy with low residuals supporting primarily MEM. Electronics Superconductors Physics applications/modelling emerge from all findings.

Keywords: Interior Optimization (IO) Methods, Critical Temperature (TC), Graphical Optimization, Systems of Nonlinear Equations

1. Introduction

Following with series of HTSCs modelling works [1, 4-6], this paper deals with 3D Graphical Optimization for development/improvement of previous research [1, 4-6]. Transition Temperature is defined as the temperature of the superconductor whose magnitude marks the beginning of superconducting effect. Critical Temperature is the optimal modelling approximation for this phenomenon because the superconducting effect occurs in experimental practice gradually, in discrete steps, or abruptly [1, 2, 4-6, 12-15, 26-29]. This research works with model T_C values which are very close to experimental literature data. Therefore, the usual Transition Temperature curves correspond to numerical fits for experimental data that have their own residual errors.

HTSCs are usually Type II ones. In BCS classical superconductors theory, the Isotope Effect model can be mathematically developed as a System of Nonlinear Equations [1, 2, 4-6, 12-15, 26-29]. Isotope Effect model 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 experimental-numerical constants, M Atomic Element Mass (AMU) of an element with (n) isotopes, T_C is critical temperature (Kelvin); (i) is the corresponding isotope for the element. This Equation (1) is the same that was set for Isotope Effect Optimization Algorithms in paper series [1, 4-6]. The modelling of T_C for any superconductor related to any parameter(s) of the material and/or external physical/chemical conditions constitutes an essential part of superconductors theory. Provided T_C be foreseeable, industrial/research applications and advances become faster and easier.

This research innovation is to apply the numerical/2D-graphical results from previous advances in [Sn-Sb-Te-Ba-Mn-Cu-O] HTSCs class. Therefore, stepping forward from [1, 4-6], the objective deals mainly with the 3D Graphical Optimization based on those calculations got in [1]. Improved 3D programming in Matlab and GNU-Octave was designed to obtain these

In summary, results are focused on MEM ILS model-programming software and computational 2D/3D imaging results both in Matlab [3D] and GNU-Octave [2D]. Specially, the 3D Graphical Optimization images obtained validate/confirm the model set in previous contributions [1,4-6].

2. Mathematical algorithms and computational data

Table 1 shows experimental data used to implement the 3D model. Equation (2) corresponds to the designed algorithm that was implemented in [1] for 2D modelling and T_C predictions. This Type II group of HTSCs modelled, [Sn-Sb-Te-Ba-Mn-Cu-O] group, whose T_C values are over 0° centigrade, forms part of recent HTSCs advances [1, 2, 4-6, 12-15, 26-29]. Numerical methods are developed from previous research [7-10, 17-25].

Table 1: The development of optimization of parameters for [Sn-Sb-Te-Ba-Mn-Cu-O] group implemented in this study [12-15]. Note the difference with the usual superconductors $T_C < 0°$

NUMERICAL OPTIMIZATION DATA FOR Sn-Sb-Te-Ba-Mn-Cu-O GROUP [HT-SUPERCONDUCTOR, MOLECULAR EFFECT HYPOTHESIS]	
FORMULATION	MOLECULAR WEIGHT (UAM) / APPROXIMATE Tc (Centigrades)
$Sn_{10}SbTe_9Ba_2MnCu_{21}O_{42+}$	+187 C
$Sn_9SbTe_8Ba_2MnCu_{19}O_{38+}$	+187 C
$Sn_8SbTe_7Ba_2MnCu_{17}O_{34+}$	+167 C
$Sn_7SbTe_6Ba_2MnCu_{15}O_{30+}$	+155 C
$Sn_{10}SbTe_4Ba_2MnCu_{16}O_{32+}$	+141 C
$Sn_9SbTe_4Ba_2MnCu_{15}O_{30+}$	+136 C
$Sn_8SbTe_4Ba_2MnCu_{14}O_{28+}$	+129 C
$Sn_9SbTe_3Ba_2MnCu_{14}O_{28+}$	+121 C

For MEM, the algorithmic constraints values are given in Table 1. This algorithm set for ILS MEM is equal to previous 2D study with this HTSCs class [1, 2, 4-6, 12-15, 26-29]. It is implemented in Matlab and GNU-Octave. Therefore, ILS formulation with a polynomial p(MO) reads,

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

where MO 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 (centigrade in this case) for every (i) member of this HTSCs group. The fig α1 is a constant specific Tikhonov Regularization Parameter. The constraints [a-b] are applied for optimization. OF was selected with ILS programming in Matlab and GNU-Octave without logaritmic-linearization, and variations depending on program result be accurate.

3. 2D/3D Numerical and graphical mem optimization results

Results are Numerical and 3D Graphical. Numerical ones include 3-degree and 4-degree ILS MEM equations. Numerical equations are shown in Tables 2,3. 2D Graphical results for 4-degree ILS polynomial model are shown with a GNU-Octave program in Fig 1. That extrapolated model-curve has an approximated parabolic shape. 3D Graphical results with Matlab for 3-degree ILS polynomial model are shown in Fig 2, 3. Matlab Graphical results for 4-degree ILS polynomial model are shown in Fig 4, 5. 2D/3D errors can be considered acceptable and low.

Numerical equations MEM

Table 2: Numerical T_C MEM for ILS 3-degree model with residual error. The software-development of parameters optimization for [Sn-Sb-Te-Ba-Mn-Cu-O] class requires appropriate patterns, loops and arrays. Setting this model in Graphs of Fig 2, 3, data obtained can be considered acceptable. Note the numerical differences with ILS 4-degree model in Table 3 in residual

ILS MOLECULAR EFFECT MODEL (3-DEGREE) WITHOUT APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
851.6384e+000	CONSTANT
-705.6519e-003	X
212.0958e-006	X^2
-19.5652e-009	X^3
RESIDUAL = 4.4432e+000	
MODEL EQUATION	
Tc = [851.6384e+000] +... ... + [-705.6519e-003] MO + ... +[212.0958e-006] MO^2 +... ...+ [-19.5652e-009] MO^3	

Table 3: Numerical T_C MEM for ILS 4-degree model with residual error and approximations [discard polynomial coefficients $\le 10^{-12}$]. The software-development of parameters optimization for [Sn-Sb-Te-Ba-Mn-Cu-O] class requires appropriate patterns, loops and arrays. Setting this model in Graphs of Fig 4, 5, data obtained can be considered acceptable. Note the numerical differences with ILS 3-degree model in Table 2 in residual

ILS MOLECULAR EFFECT MODEL (4-DEGREE) WITH APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
-19.7073e+003	CONSTANT
20.3783e+000	X
-7.8396e-003	X^2
1.3374e-006	X^3
≈ 0	X^4
RESIDUAL = 4.2910e+000	
MODEL EQUATION	
Tc = [-19.7073e+003] +... ... + [20.3783e+000] MO + ... +[-7.8396e-003] MO^2 +... ...+ [1.3374e-006] MO^3	

2D Graph MEM 4 Degrees

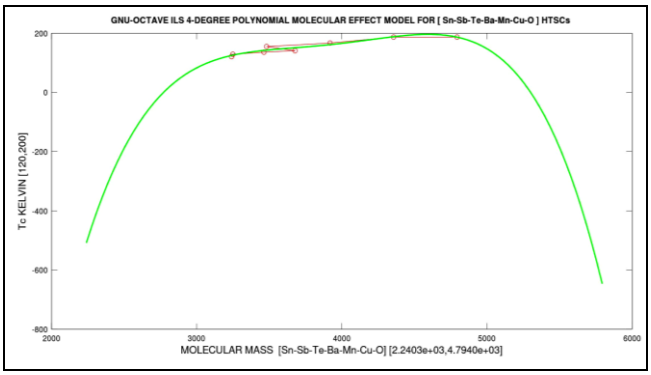

Fig1: GNU-OCTAVE 4-degree ILS polynomial optimization of Molecular Effect Model for [Sn-Sb-Te-Ba-Mn-Cu-O] HTSCs group. Extrapolated modelled curve (green) and experimental data (red). The model is a parabolic equation, approximately. The numerical results with acceptable residuals were presented in previous article [1, 2, 4-6, 12-15, 26-29].

3D Graphs MEM 3 degrees

Fig 2, 3 present imaging results for ILS 4-Degree MEM. Fig 3, Imaging Processing method 1, shows a 3D Graphical Optimization example. That is, T_C experimental (Y axis) and T_C MEM predicted (Z axis).

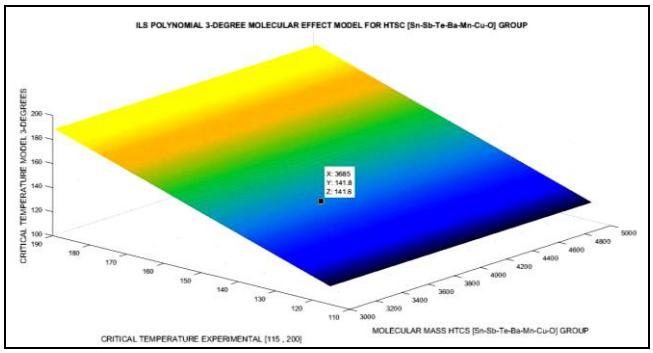

Fig 2: 3-Degree polynomial MEM 3D graph showing model T_C prediction and 3D experimental data which are equal—shown inset with Matlab cursor data. At Z axis MEM data with imaging processing method 1. Matrices for 3D Graphical Optimization are [500 x 500]

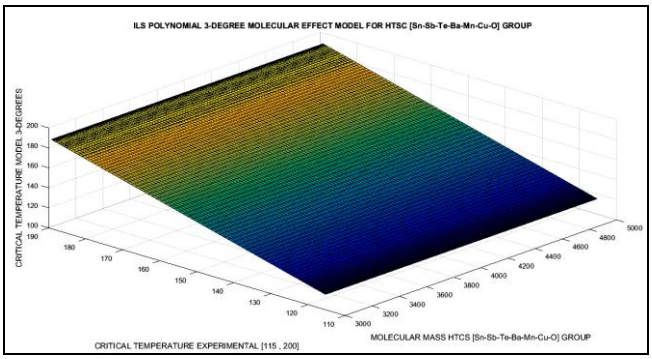

Fig 3: 3-Degree polynomial MEM 3D graph showing model T_C prediction and 3D experimental data which are equal. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are approximately [250 x 250]

4D Graphs MEM 4 degrees

Fig 4,5 present imaging results for ILS 4-Degree MEM. Fig 3, Imaging Processing method 1, shows a 3D Graphical Optimization example. That is, T_C experimental (Y axis) and T_C MEM predicted (Z axis).

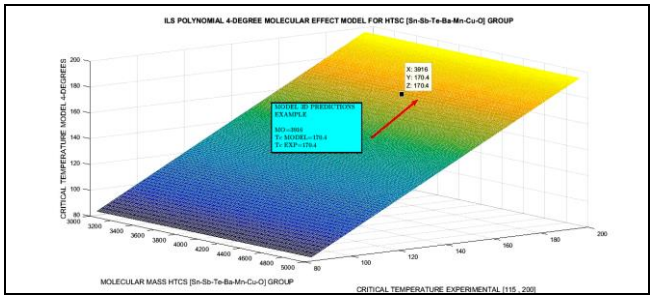

Fig 4: 4-Degree polynomial MEM 3D graph showing model T_C prediction and 3D experimental data which are equal. At Z axis MEM data with imaging processing method 1. Matrices for 3D Graphical Optimization are [250 x 250]

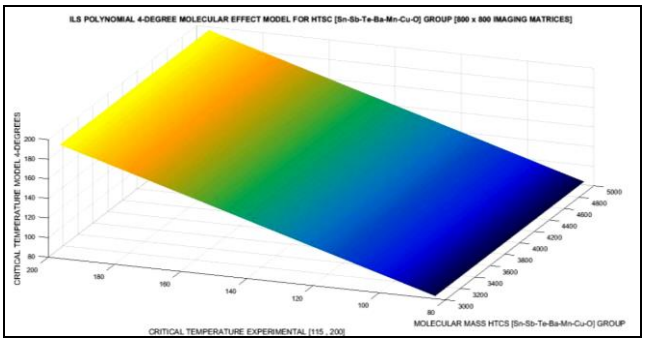

Fig 5: - 4-Degree polynomial MEM 3D graph showing model T_C prediction and 3D experimental data with [800 X 800] imaging matrices. At Z axis MEM data with imaging processing method 1. Y axis T_C experimental and X axis Molecular Mass. Imaging processing method 1. Delaunay tiles number increases and the MEM surface becomes smoother and almost continuous.

4. Discussion and conclusions

The objective of this study was to develop the 2D results from [1] towards a 3D Graphical Optimization of MEM for [Sn-Sb-Te-Ba-Mn-Cu-O] HTSCs class. Results parts can be classed into numerical and 3D graphical. Numerical results for this HTSC group MEM can be considered acceptable with low residuals. The estimates with 3- and 4-degree ILS polynomial methods solutions are useful for T_C extrapolations. Both Matlab and GNU-Octave systems were used for getting equations and charts.

MEM is a hypothesis coming from the Isotope Effect physical-chemical concepts. Its equations and parameters are in development [1]. From its fundamentals, it is cautiously/primarily guessing the phenomena that may occur when deviations of molecular mass caused by proportion/isotopic-variation in the molecule happen. Therefore, for those physical-chemical and thermodynamic-electronics environments it may/could exist a mathematical model to predict the T_C magnitude change for every HTSCs class.

Numerical equations in 3 and 4 ILS polynomial degrees show be accurate with low residuals. 2D/3D Graphical Optimization results both in Matlab and GNU-octave are considered acceptable. Software improvements with specific subroutines and patters resulted in two model ILS fomulas and clear/ satisfactory images.

In conclusion, 2D/3D ILS Graphical Optimization methods have verified the primary theoretical hypothesis for MEM in

[Sn-Sb-Te-Ba-Mn-Cu-O] HTSCs class. Further research will continue to improve hypothesis/formulation MEM initial steps.

5. Scientific ethics standards

Molecular Effect Model (MEM), was created by author in 2020-1. 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 Francisco Casesnoves in 2020. This article has previous papers information, from [1, 4-6, 7-10, 17-25], whose inclusion is essential to make the contribution understandable. The article has data and algorithm formulas from [1], which is essential for MEM equations and 3D modelling. 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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