International Journal of Scientific Research in Computer Science, Engineering and Information Technology
ISSN : 2456-3307 (www.ijsrcseit.com)
doi : https://doi.org/10.32628/CSEIT228340

Mathematical 3D Graphical Optimization with Review of 2D Optimization Methods for Molecular Effect Model in High Temperature Superconductors Tl Class [$T_C > 0°$]

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Article Info
Volume 8, Issue 3
Page Number : 176-184

Publication Issue :
May-June-2022

Article History
Accepted: 10 May 2022
Published: 30 May 2022

ABSTRACT

Following High Temperature Superconductors (HTCSs) study series, Inverse Least Squares (ILS) 2D/3D Numerical/Graphical Optimization for Molecular Effect Model (MEM) in group of [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O], with [$T_C > 0°$], is developed. Additionally, a laboratory results-review of 2D/3D Optimization methods for this HTSCs class is included exclusively for [$T_C > 0°$]. Solutions with 3D Graphical Optimization techniques to validate primarily the MEM are presented. Results comprise 2D/3D Tikhonov Regularization algorithms with mathematical methods for this class. Findings obtain acceptable Numerical and 2D/3D Graphical Optimization outcomes with low error-residuals. Results show two parts, the 3D Graphical Optimization MEM modelling and a review of 2D/3D Graphical Optimization findings. Electronics Physics applications for Superconductors and HTSCs are extrapolated.

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), Molecular Effect Model (MEM) .

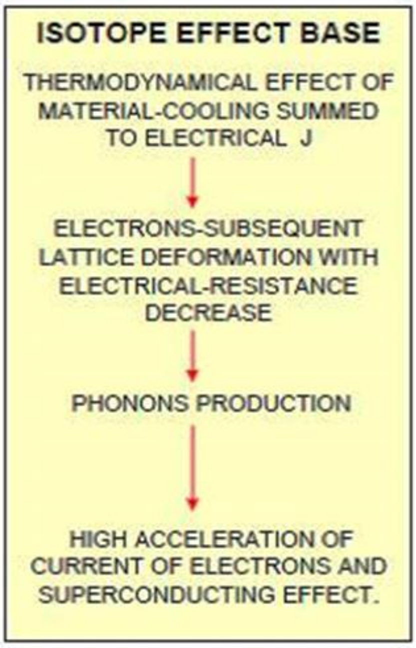
I. INTRODUCTION

Continuing the Molecular Effect Modelling series for HTSCs classes, [1,4-6, 42], 3D Graphical Optimization of the group [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] whose $T_C > 0°$ centigrades is developed. This recent Type II HTSCs materials-class, shows T_C magnitudes both over and under 0 ° Centigrade [3-5, 12-15, 32-34, 37, 42]. That is its particular thermodynamical-materials difference compared to other HTSCs groups.

Sketch 1 shows the Isotope Effect physical-chemical base [3-5, 12-15, 32-34, 37, 42]. Along these contribution series, MEM [Casesnoves, 2020,1,4-6, 42], constitutes an extrapolation of this theoretical background. In superconductors theory and HTSC modelling, Electronics-Materials Physics, Chemistry, Thermodynamics, and Quantum Mechanics, among others, converge to form the models and base of the theorical/experimental foundation.

A previous article presented primary optimization for other class of HTSCs with $T_C > 0°$ centigrade [1,42]. As usual, [1-6, 14-16, 26-29, 42], the critical temperatures magnitude interval for HTSCs begins with those superconducting materials whose Tc is approximately higher than 77 K.

This study deals with 2D/3D Graphical/Numerical-Algorithms MEM for HTSCs [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] class. The MEM temperature-range constraint for optimization is set to compounds whose $T_C > 0°$.



Sketch 1.- Basic physical-chemical process for Isotope Effect phenomena [3-5, 12-15, 32-34, 37, 42] . MEM idea was extrapolated from this theory.

Along a publications series in this line, [3-5, 12-15, 32-34, 37, 42] the programming BCS formula implemented for Isotope Effect model was a System of Nonlinear Equations algorithm. For uni-element superconductors this equation, [1,4-6,42], reads,

$$[M_i]^{\alpha} T_C - K \cong 0 ;$$
$$\text{for } i = 1, \ldots, n ; \qquad (1)$$

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, in this study Centigrade); (i) is the corresponding isotope for the element.

The [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] class whose molecular composition/formulation differs in proportion of valences/elements, Table 1, is 2D/3D numerically/graphically optimized with ILS polynomial MEM method [1,42]. Results show be acceptable both numerically and graphically. Software was designed based on previous improvements [1,4-6,42] .

Concisely, the article shows a 2D/3D Numerical-Graphical Optimization study heading for the primary MEM hypothesis developed for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs class. Programming-algorithms are implemented with Matlab imaging-processing software and 2D Laboratory Reviews graphical model plots are presented. MEM shapes resemble approximately sinusoid-like curves.

II. MEM MATHEMATICAL ALGORITHMS AND EXPERIMENTAL DATA

The objective approached is to design 3D MEM based on experimental data, Table 1. As it was previously explained, [3-5, 12-15, 26-29, 32-34, 37, 42] for scientific clarity, the inclusion of the algorithm development [1,42] is set in this section. The Type II HTSCs class is [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] whose Tc values are higher/lower than 0° centigrade. Table 1 presents the molecular chemical-physical data for 3D Graphical and Numerical Optimization. Particular characteristic of this HTSCs class is the finding of clear 3D imaging zones that separate the positive values of Tc from the negative ones in MEM.

NUMERICAL OPTIMIZATION DATA [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] CLASS [HT-SUPERCONDUCTORS, [Tc > 0°] MOLECULAR EFFECT HYPOTHESIS]	
FORMULATION	MOLECULAR WEIGHT (UAM) / APPROXIMATE Tc (CENTIGRADES)
Tl7Sn2Ba2MnCu10O20	2.9531e+03 / 77
Tl7Sn2Ba2TiCu10O20	2.9461e+03 / 65
Tl6Sn2Ba2TiCu9O18	2.6462e+03 / 56
Tl7Sn2Ba2SiCu10O20	2.9263e+03 / 53
Tl6Ba4SiCu9O18	2.6636e+03 / 48
Tl5Ba4SiCu8O16	2.4479e+03 / 44
(Tl5Sn2)Ba2SiCu8O16	2.3264e+03 / 42
(Tl5Pb2)Ba2SiCu8O16	2.5034e+03 / 38
(Tl5Pb2)Ba2Si2.5Cu8.5O17	2.5933e+03 / 35
(Tl5Pb2)Ba2Mg2.5Cu8.5O17	2.5839e+03 / 30
(Tl5Pb2)Ba2Mg2Cu9O18	2.6195e+03 / 28
(Tl5Pb2)Ba2MgCu10O20	2.6907e+03 / 18
(Tl4Pb)Ba2MgCu8O13	2.0401e+03 / 3

Table 1.- The development data for optimization of parameters for Graphical/Numerical-Algorithms MEM in HTSCs [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] group implemented—without subscript valences figures for clarity. This method was used in previous studies with different HTSCs materials [1,42].

From [1,4-6, 42], MEM parameters and constraints are set in a Nonlinear Tikhonov algorithm. This algorithm is the base of the series of studies in HTSCs modelling. The same formula with programming variations implemented for ILS MEM, with a polynomial p(MO) reads,

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

where, as [1,4-6, 42], 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 HTSCs group. The figure α1 is a constant specific Tikhonov Regularization Parameter. The constraints [a-b] are applied for optimization. OF was done without algorithmic-linearization.

III. 3D MEM ILS OPTIMIZATION RESULTS

The 3D MEM Graphical implementation is shown in Figures 1,2,3. The 2D review of MEM laboratory data for ILS polynomial algorithm 3,4,5 degrees is presented in Figures 4,5,6. Both 3D/2D results get numerical/graphical solutions with acceptable residuals. The steady sinusoid-shape of MEM in all types of ILS 2D curves validates the findings. It corresponds sharply to this HTSCs class that could have Tc magnitudes higher and lower than 0 ° Centigrade. Time consuming for running program is about 5-10 seconds, depending on graphics options and matrices size. The 2D section comprises laboratory data review for this MEM [1,42].

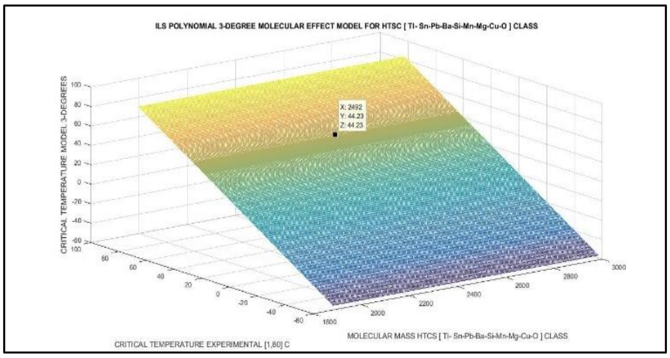


Fig. 1.- 3-Degree polynomial MEM 3D graph showing model Tc prediction and 3D experimental data which are approximately equal. Numerical example coincidence between experimental and MEM data is marked. Note the dark zone at surface that means the transition between negative and positive Tc for the MEM. This matches the 2D results of Figures 3,4,5. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are [300 x 300].

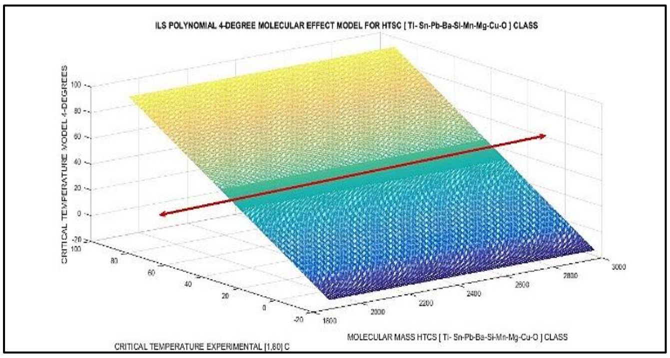


Fig. 2.- 4-Degree polynomial MEM 3D graph showing model Tc prediction and 3D experimental data which are approximately equal. Note the clearer zone at surface with red arrow that means the transition between negative and positive Tc for the MEM. This matches the 2D results of Figures 3,4,5. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are [300 x 300].

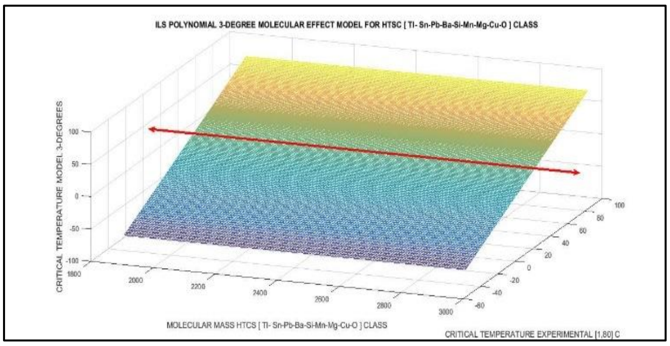


Fig. 3.- Different perspective for 3-Degree polynomial MEM 3D graph showing model Tc prediction and 3D experimental data which are approximately equal. Note the dark zone at surface over the red arrow that means the transition between negative and positive Tc for the MEM. This matches the 2D results of Figures 3,4,5. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are [300 x 300]. Enhanced in Appendix.

IV. REVIEW 2D/3D GRAPHICAL OPTIMIZATION MEM RESULTS

2D Laboratory imaging/numerical data review is presented in Figures 4,5,6. ILS polynomial with 3,4 and 5-degree show a sinusoid curve-shape for MEM. 2D Graphical errors can be considered acceptable/low.

ILS Review of 3,4,5-Degree Graphical Optimization Model Results

Figures 3,4,5 show sinusoid-shaped model curve for ILS 3,4,5-degree Molecular effect model in [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. There is a clear variance in shape compared to parabolic model-curves obtained in previous studies with different HTSCs class [1, 4-6, 42].

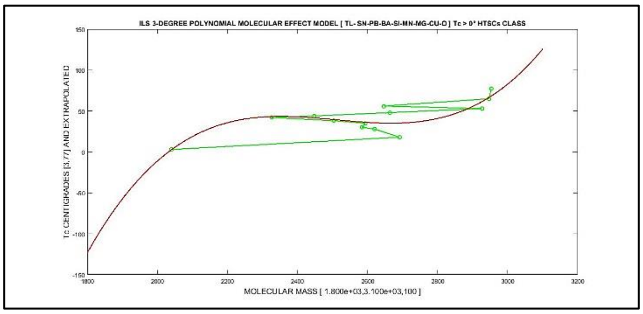


Fig. 4.- Approach with 3-degree ILS MEM polynomial optimization for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. Matlab Extrapolated modelled curve (red) and experimental data (green). MEM results to resemble a sinusoid-like curve, approximately. Since this HTSCs class has a number of compounds with Tc < 0° , MEM confirms that affinity.

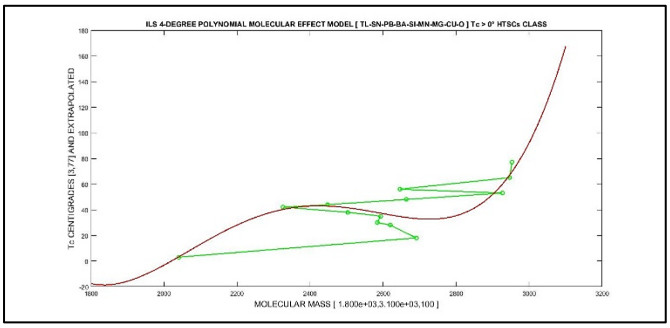


Fig. 5.- Approach with 4-degree ILS MEM polynomial optimization for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. Extrapolated modelled curve (red) and experimental data (green). MEM results to resemble a sinusoid-like curve, approximately. Since this HTSCs class has a number of compounds with $T_C < 0°$, the model confirms that affinity matching shape of Figure 4. A clear contrast in shape compared to parabolic model-curves obtained in previous studies with different HTSCs class [1, 4-6, 42].

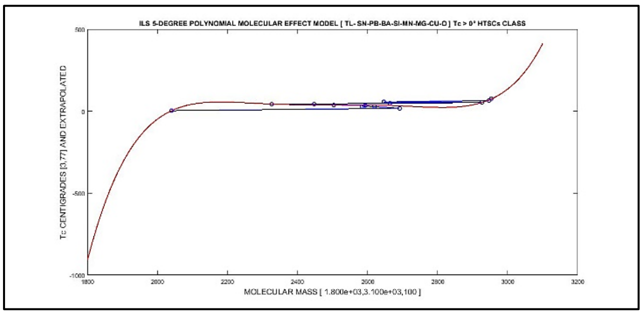


Fig. 6.- Approach with 5-degree ILS MEM polynomial optimization for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group. Extrapolated modelled curve (red) and experimental data (blue). MEM results to resemble a sinusoid-like curve, approximately. Since this HTSCs class has a number of compounds with $T_C < 0°$, MEM confirms that affinity. Note the almost linear part of the model curve.

V. DISCUSSION AND CONCLUSIONS

The objective of this study was to get a 3D Graphical/Numerical Optimization MEM for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs class constrained to $T_C > 0°$ C. For this HTSCs group, review of previous laboratory results in 2D that confirm a sinusoid-shape of MEM were also presented. T_C experimental magnitudes for [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs class have been extrapolated with the model for under/above 0° C thermodynamical conditions.

The HTSCs class has experimental T_C values over/under 0° C, and the algorithm/program was designed exclusively for $T_C > 0°$ C. Therefore, MEM approach seemed be specially complicated. Instead of what was supposed be a hurdle for this HTSCs class modelling, the sinusoid MEM shape is found for all degree-types of MEM equations, and covers T_C magnitudes under/above 0° C.

Thus, results have two strands, 3D Graphical and Numerical ones, and 2D MEM curve series. 3D Graphical Optimization graphs can be considered acceptable with low residuals. 2D curves for 3,4 and 5 degrees of polynomial MEM coincide in sinusoid-like shape.

Succinctly, 3D Graphical and Numerical Optimization and 2D ILS polynomial-modelling Graphical Optimization methods for HTSCs group [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] were approached with acceptable results. Applications in Electronics Physics become from the 3D/2D Numerical/Graphical study findings.

VI. SCIENTIFIC ETHICS STANDARDS

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, whose inclusion is essential to make the contribution understandable. The 2D Graphical Optimization in Matlab and GNU-Octave constitutes a software engineering improvement from previous contributions [1,4-6,42]. 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 European Union Technology and Science Ethics. Reference, '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 [38-41]. 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, proposition or theorem is presented, demonstration is always included. 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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VIII. AUTHOR'S BIOGRAPHY

Dr Francisco Casesnoves earned the Engineering and Natural Sciences PhD by Talllinn University of Technology (started thesis in 2016, thesis Defence/PhD earned in December 2018, official graduate Diploma 2019). He works as independent research scientist in computational-engineering/physics. Dr Casesnoves earned MSc-BSc, Physics/Applied-Mathematics (Public Eastern-Finland-University, MSc Thesis in Radiotherapy Treatment Planning Optimization, which was developed after graduation in a series of Radiation Therapy Optimization-Modelling publications [2007-present]). Dr Casesnoves earned Graduate-with-MPhil, in Medicine and Surgery [1983] (Madrid University Medicine School, MPhil in Radioprotection Low Energies Dosimetry [1985]). He studied always in public-educational institutions, was football player 1972-78 (defender and midfielder) and as Physician, supports healthy life and all sports activities. Casesnoves resigned definitely to his original nationality in 2020 for ideological reasons, democratic-republican ideology, and ethical-professional reasons, and does not belong to Spain Kingdom anymore. His constant service to the International Scientific Community and Estonian technological progress (2016-present) commenced in 1985 with publications in Medical Physics, with further specialization in optimization methods in 1997 at Finland—at the moment approximately 100 recognized publications with approximately 62 DOI papers. His main branch is Computational-mathematical Nonlinear/Inverse Methods Optimization. Casesnoves best-achievements are the Numerical Reuleaux Method in dynamics and nonlinear-optimization [books 2019-2020], The series of Radiotherapy Improvements for AAA superposition-convolution model, the Graphical and Interior Optimization Methods [2016-8], the new Computational Dissection-Anatomical Method, [2020], invention of Forensic Robotics [2020-2021], and Molecular Effect Model for High Temperature Superconductors [2020]. Dr Casesnoves scientific service since 2016 to the Free and Independent Republic of Estonia for technological development (and also at Riga technical University, Power Electrical and Electronics Department) is about 37 physics-engineering articles, two books series, and 1 industrial radiotherapy project associated to Europe Union EIT Health Program (Tartu University, 2017).

Cite this article as :

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Journal URL : https://ijsrcseit.com/CSEIT228340

APPENDIX

Fig. 3 [Enhanced].- Different perspective for 3-Degree polynomial MEM 3D graph showing model TC prediction and 3D experimental data which are approximately equal. Note the dark zone at surface over the red arrow that means the transition between negative and positive TC for the MEM. This matches the 2D results of Figures 3,4,5. At Z axis MEM data with imaging processing method 2. Matrices for 3D Graphical Optimization are [300 x 300].