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3D Graphical Optimization for Molecular Effect Model in High Temperature Superconductors Thallium Class [$T_C < 0°$, $T_C > 0°$] without Lattice Tetragonal Compounds

Francisco Casesnoves *1

*1 PhD Engineering, MSc Physics-Mathematics, Physician. Independent Research Scientist. International Association of Advanced Materials, Sweden. Uniscience Global Scientific Member, Wyoming, USA.
casesnoves.research.emailbox@gmail.com 1

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ABSTRACT

In subsequent study series for 3D High Temperature Superconductors (HTCSs), Inverse Least Squares (ILS) and 3D Numerical/Graphical Optimization is the objective for this Molecular Effect Model (MEM) contribution. HTSCs class selected is Thallium group of [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O], constrained/extended to [$T_C < 0°$, $T_C > 0°$]. Tetragonal Lattice and Amorphous compounds of this Type II Thallium HTSCs class are not included in this study. Results obtained for Matlab 3D Graphical Optimization techniques are proven/presented. Numerical calculations include 3D Tikhonov Regularization algorithms with mathematical developments for this Thallium class. Thus, results show two strands, 3D surfaces for Graphical Optimization MEM Thallium HTSCs modelling, and MEM analysis of numerical equations. 3D MEM and Numerical Optimization get low error and residuals. Electronics Physics applications emerge from allteh research.

Keywords : Interior Optimization (IO) Methods, Graphical Optimization, Systems of Nonlinear Equations, Tikhonov Regularization (TR), Critical temperature [Tc], Inverse Least Squares (ILS), Electronics Superconductors (SC), 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), Superconducting Multifunctional Transmission Line (SCMTL).

I. INTRODUCTION

The research paper develops 3D Molecular Effect Modelling in HTSCs Thallium class, [1,4-6, 42-46] to continue with HTSCs MEM series findings. 3D Graphical Optimization of the Thallium class [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] with [$T_C < 0°$, $T_C > 0°$] is presented as a forward research from [46].

Sketch 1 shows concise of the HTSCs 2D series results for MEM analytic geometry. Parabolic shapes are dominant along all MEM research, [1,4-6, 42-46] . The most perfect MEM 2D analytic geometry corresponds to Thallium HTSCs class sigmoid curves, Appendix.

Therefore, the contribution presents 3D Graphical Optimization extension from MEM numerical data of HTSCs Thallium class, subject to [$T_C < 0°$, $T_C > 0°$]. Amorphous Thallium compounds and Tetragonal Lattice compounds experimental database are not included at T_C interval, Tables 1-2. Specific Matlab programs, Sketck 2, were got with imaging processing subroutines, patterns, loops, and imaging processing subroutines combinations.

Succintly, the article shows a Matlab, 3D Numerical-Graphical Optimization research for MEM in HTSCs [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Thallium class. Algorithms and programming methods are explained sharply. Electronics Physics applications are detailed in [42-46].

MEM ANALYTIC GEOMETRY CHARACTERISTICS FOR HTSCs GROUPS	
HTSC CLASS	**2D MEM GEOMETRY**
Cuprates [Hg-Ba-Ca-Cu-O]	Parabolic approximated [focus inverse y-axis]
Sn Class [Sn-Sb-Te-Ba-Mn-Cu-O]	Parabolic approximated [focus inverse y-axis]
Thallium Class [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O]	Sigmoid sharp At any MEM polynomial optimization All temperature intervals without TET Lattice compounds
Pb Class	Parabolic approximated [focus x-axis]

Sketch 1.-Accrding to HTSCs MEM publications series, [1,4-6, 42-46], the results of analytic geometry MEM optimization.

II. MEM MATHEMATICAL ALGORITHMS AND EXPERIMENTAL DATA

As in [46], MEM computational method experimental database and programming algorithm is shown in Tables 1-2. The corresponding program structure is presented at Sketch 2. Optimization formulas/algorithms are built based on Tikhonov Regularization Theory [7,13,31,42,43,44,45,46], Equation 1. Table 1 describes numerical experimental data implemented for MEM [4-6, 12-15, 32-34, 37, 42-46] for $T_c > 0°$ Celsius. Table 2 shows Numerical Experimental Data implemented for MEM [4-6, 12-15, 32-34, 37, 42-46] for $T_c < 0°$ Celsius.

Table 1.- Literature experimental data for Thallium class constrained to [$T_C > 0°$], [7,13,31,42,43,44,45,46]. Optimization of parameters in 3D Graphical/Numerical-Algorithms MEM for HTSCs Thallium group are set with this numbers, adding data from Table 2. This experimental database corresponds to former research series with different/extended critical temperature range [43-46].

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

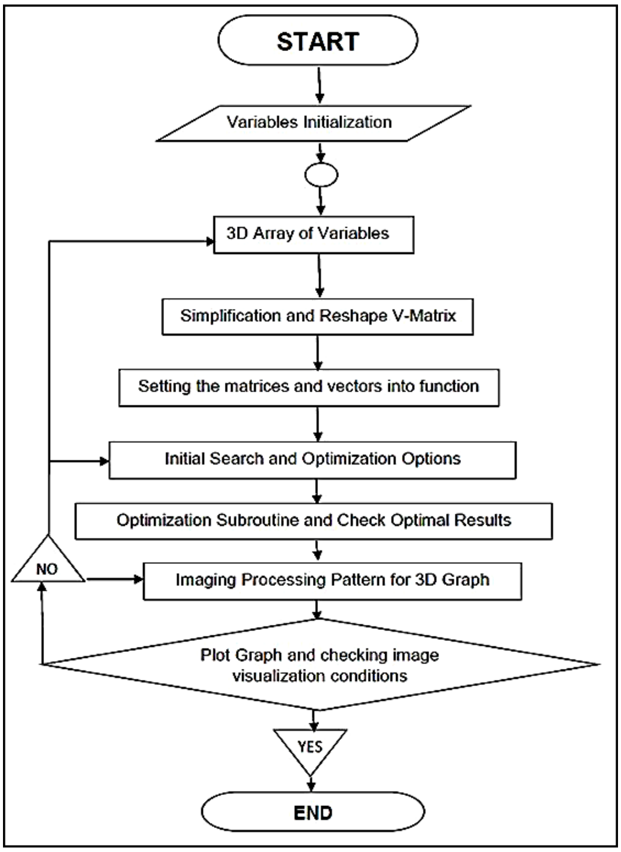
Table 2.- Experimental dataset for optimization to include compounds whose [Tc < 0°] . Optimization parameters in 3D Graphical/Numerical-Algorithms MEM for HTSCs Thallium group are shown in Equation 1.

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)
(Tl4Ba)Ba2MgCu8O13	1.9702e+003 / -8
(Tl4Ba)Ba2Mg2Cu7O13	1.9309e+003 / -15
(Tl4Ba)Ba2Ca2Cu7O13	1.9625e+003 / -19

MEM formulas/algorithms from [1,4-6, 12-15, 32-34, 37, 42, 43, 44,45, 46] are implemented in Matlab software. As in [46], Equation (1) describes Inverse Tikhonov functional method like [42, 43, 44, 45, 46]. Hence, ILS Inverse Tikhonov algorithm MEM, with a polynomial p(MO) reads.

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

where, as developed in [1, 4-6, 42, 43, 44,45,46], MO is HTSC molecular mass of the HTSC selected (i) within a HTSC group with (i) elements and [a-b] are numerical constraints interval vectors. T_{Ci} is every critical temperature (Centigrade for MEM Thallium HTSCs class) for each (i) member of HTSCs class. The parameter α1 is a specific constant for Inverse Tikhonov Regularization. Constraints, related to Tc and MO values from experimental data, Tables 1-2, are set in a vector interval [a-b].



Sketch 2.-Basic software method to implement Equation (1) for 3D Thallium MEM optimization.

III. RESULTS

3D MEM Graphical implementation with [Tc < 0° , Tc > 0°] is shown in Figures 1,2. It follows study from [46], whose 2D fitting results obtained for MEM numerical/graphical proved acceptable residuals. 3D images confirm the 2D MEM Thallium solutions [46]. Programming time for getting images is about 6-10 seconds. The higher number of subroutines combinations, the more running time for image processing. Appendix shows a comparative MEM image with 2D sigmoid curves got in [46]. Software matrices size vary within interval [200x200 , 400x400].

3D GRAPHICAL OPTIMIZATION RESULTS [$T_C < 0°$, $T_C > 0°$]

3D series of images for Thallium class with [$T_C < 0°$, $T_C > 0°$] numerical data implemented [43-46] are presented in Figures 1-2. 2D images numerical data match the 3D ones.

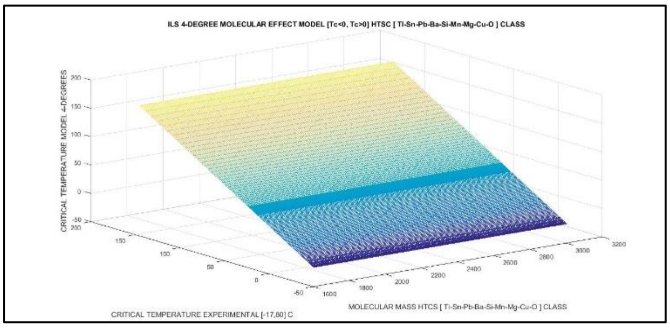


Fig. 1.- 3D Matlab imaging processing with 4-Degree ILS MEM polynomial optimization for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs Thallium class, [$T_C < 0°$, $T_C > 0°$] . As in [46], this HTSCs class numerical data has a number of compounds with [$T_C < 0°$] , MEM verifies [46] numerical results by using image processing cursor. Enhanced at Appendix.

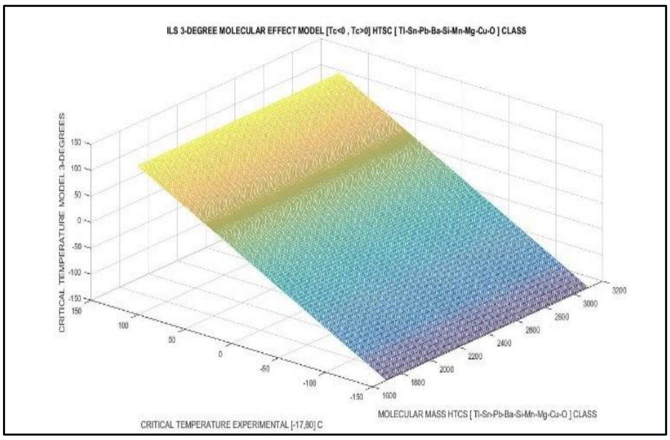


Fig. 2.- 3D Matlab imaging processing with 3-Degree ILS MEM polynomial optimization for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs Thallium class, [$T_C < 0°$, $T_C > 0°$] . As in [46], this HTSCs class numerical data has a number of compounds with [$T_C < 0°$] , MEM verifies [46] numerical results by using image processing cursor. Dark surface strip denotes the transition from [$T_C > 0°$] to [$T_C < 0°$] .

IV. DISCUSSION AND CONCLUSIONS

The research objectives were stepping forward from 2D, [46], to 3D graphical Optimization. That is, to get a Matlab 3D Graphical/Numerical Optimization MEM for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs Thallium class at [$T_C < 0°$, $T_C > 0°$] centigrades T_C interval. All the software series of 3D graphs were designed to demonstrate the increasing correctness of the MEM fitness provided at [$T_C < 0°$, $T_C > 0°$] Centigrade.

The 3D Graphical and Numerical Optimization, Figures, 1,2, prove the 3D MEM accuracy that was developed in 2D at [46]. Results corroborate the findings of previous studies [43,44,45,46].

In summary, 3D Matlab MEM Graphical Optimization imaging processing confirms 2D MEM results from [46]. The T_C interval was extended along range [$T_C < 0°$, $T_C > 0°$] centigrade without TET Lattice compounds. Applications in Electronics Physics in HTSCs Type II can be guessed from the research.

V. SCIENTIFIC ETHICS STANDARDS

The Molecular Effect Model base was set by Dr F Casesnoves on 15th March 2022. All the papers series of Superconductors and HTSCs are different in text, images (unless an image citation is necessary), programming applied and conclusions. Usually every Superconductor or HTSC element/class study starts with previous 2D optimization and steps up to 3D optimization in subsequent study/articles. Basic algorithms are used in series with equal structure but different parameters magnitudes/intervals. IMPORTANT NOTE: In previous publication with Matlab, [43], a printing mistake in polynomial constant is the default of negative sign. The correct value is [-8.2906e+03] , and NOT like in [43], [+8.2906e+03]. Equation 1 is the algorithms used in HTSCs series study [43,44,45,46], and cannot be written differently. Matlab software is original from the author in all 2D/3D and Numerical Optimizations results presented [46]. 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/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. 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, lobbies of any kind, religious-similar, non-scientific theories, personal opinions, political ideas, friends or relatives favours, 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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Journal URL : https://ijsrcseit.com/CSEIT228430

VII. AUTHOR'S BIOGRAPHY

Dr Francisco Casesnoves earned the Engineering and Natural Sciences PhD by Tallinn University of Technology (started thesis in 2016, thesis Defence/PhD earned in December 2018, official graduate Diploma 2019). Dr Casesnoves is European Union and Internationally qualified as Doctor in Engineering to supervise PhD Theses, Master Theses, and Bachelor Theses in science and engineering. 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, ethical-professional reasons, anti-state monarchy corruption positions, 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 70 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], Molecular Effect Model for High Temperature Superconductors [2020], and Superconducting Multifunctional Transmission Line [2021-2]. Dr Casesnoves PhD thesis is an Estonian scientific service to European Social Fund and several EU Research Projects. 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 40 physics-engineering articles, two books series, and 1 industrial radiotherapy project associated to Europe Union EIT Health Program (Tartu University, 2017).

APPENDIX

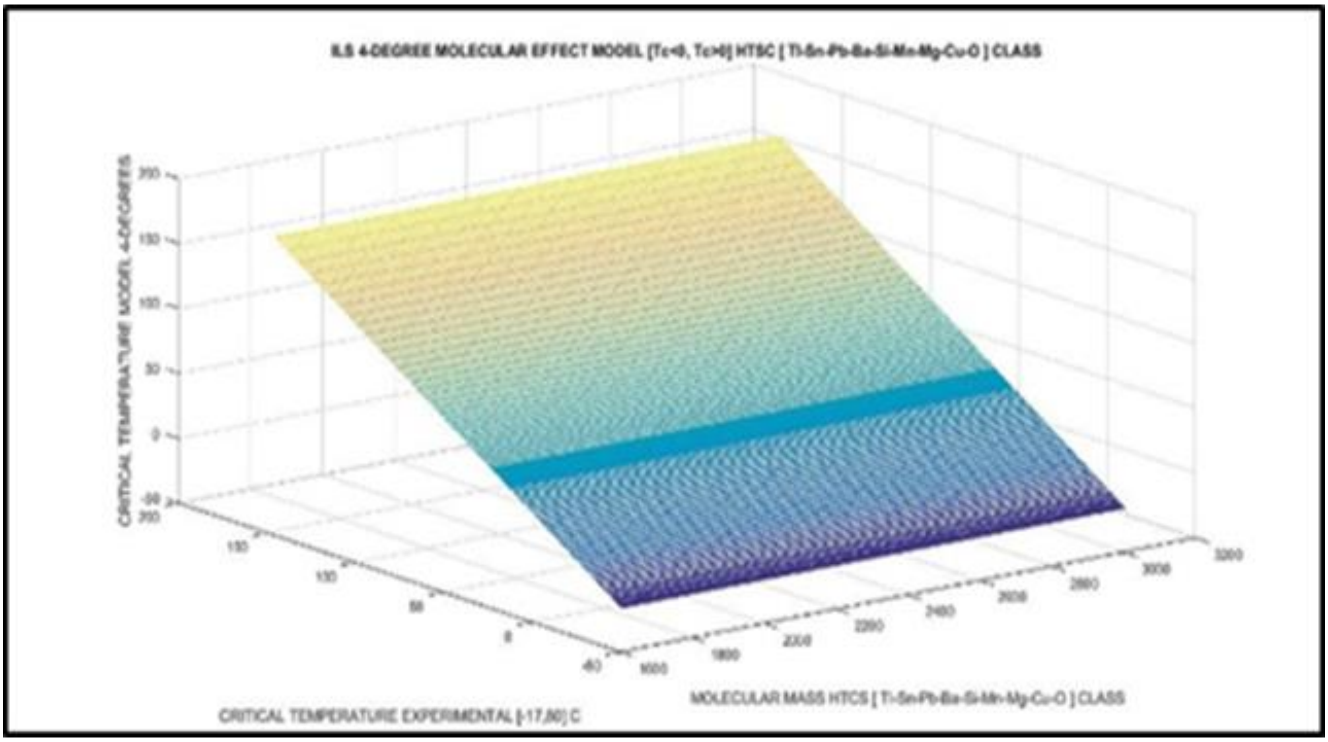
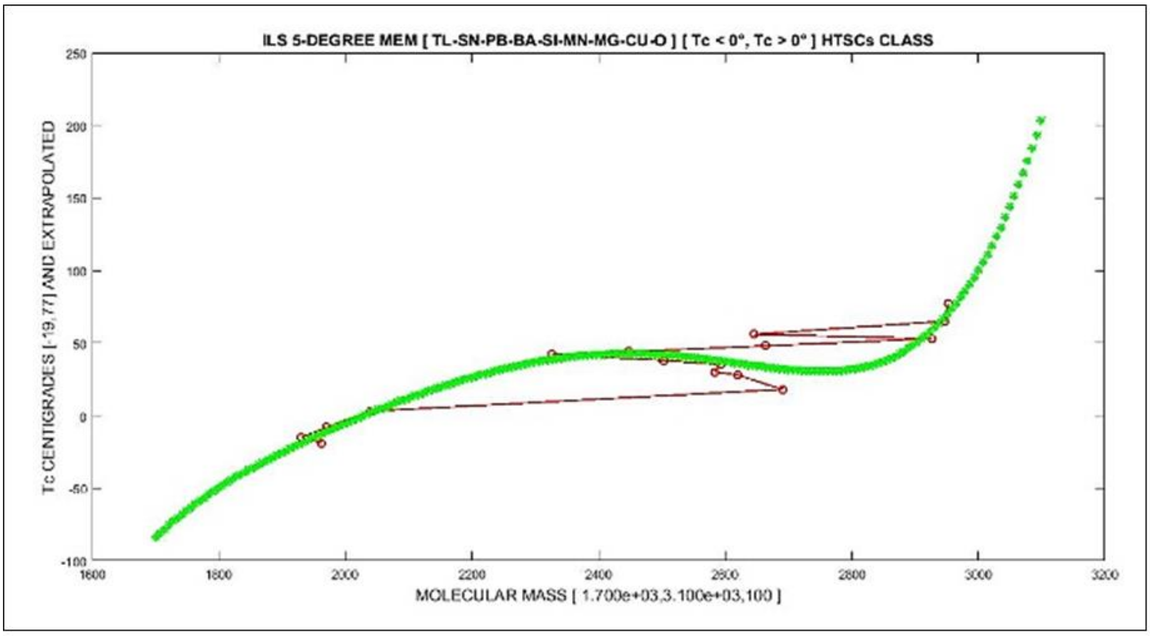


Fig. 1 [enhanced].- 3D Matlab imaging processing with 4-Degree ILS MEM polynomial optimization for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs Thallium class, [$T_C < 0°$, $T_C > 0°$] . As in [46], this HTSCs class numerical data has a number of compounds with [$T_C < 0°$] , MEM verifies [46] numerical results by using image processing cursor.



Comparative Fig. 3 from [46].- 2D analytic geometry sigmoid demonstration. The most accurate approach although rather a large polynomial equation [43-46]. Matlab imaging processing with 5-Degree ILS MEM polynomial optimization for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs Thallium class, [$T_C < 0°$, $T_C > 0°$] . Modelled curve (green) and experimental data (red). MEM results to confirm a sinusoid-like curve, just like in [43-46], approximately. Since this HTSCs class numerical data has a number of compounds with [$T_C < 0°$], MEM verifies that analytical geometry.