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Optimization of Critical Temperature Molecular Effect Model Predictions Series with 2D Graphical Statistics for High Temperature Superconductors Thallium Class [$T_C < 0°$, $T_C > 0°$]

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Abstract

In High Temperature Superconductors (HTCSs) Molecular Effect Model (MEM) publication series, Critical Temperature Inverse Least Squares Predictions (ILS) with 2D Numerical/Graphical Optimization in Thallium group of [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] are shown. These approximations are constrained for selected compounds with [$T_C < 0°$, $T_C > 0°$]. Tetragonal Lattice and Amorphous compounds of this Thallium class are not included yet. Results, additionally, comprise a 2D Statistics Graphics series subject to these conditions with 97% Confidence Intervals. Solutions and low errors with 2D Numerical Optimization techniques to validate the MEM for this class are presented. 2D Graphical-Statistical results comprise 97% confidence interval approximations. Electronics Physics applications for Superconductors in general, and HTSCs are described.

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

Introduction

This subsequent research study follows the series of publications in Superconductors (SCs) and High Temperature Superconductors (HTSCs) for critical temperature [Tc] modelling optimization [1, 4-6, 42, 43, 44]. The model used is Molecular Effect Model (MEM). The objective in this paper is to develop MEM statistical graphs/results, show numerical equations explicitly for several polynomial degrees of MEM, and calculate T_C numerical predictions with this data.

In the HTSCs Thallium class [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] the atomic mass of every element could vary in function of the selected isotope. For example, Thallium atomic mass could fluctuate approximately from 176 to 216 depending on the type of isotope theoretically selected for the HTSC molecule. Other molecular elements, such as Barium, Copper or Oxygen, can also differ in AMU. Additionally, although the isotopes atomic mass differences could be small, the valences in this HTSC class are so high that it can create a change/variation in molecular weight. Other reason is that new upcoming compounds of Thallium class whose molecular mass might be within this interval could be subject for this approximate T_C predictions type [14-16, 26-29, 32-34, 44-47].

Therefore, what is meant in this study is to obtain approximate numerical predictions for T_C with the optimal equations and 2D graphics previously calculated. Numerical predictions are useful both for current sc-materials and prospective ones. In this research, MATLAB system is applied to achieve 2D Graphical Optimization, ILS Numerical Equations, and T_C MEM Predictions Tables. The study improvement is that MEM covers T_C data for [$T_C < 0°$, $T_C > 0°$]. Comparisons to previous contributions are evaluated [1, 4-6, 42, 43, 44].

Concisely, this continuing article provides a MATLAB system 2D Numerical-Graphical optimization research for MEM in HTSCs Thallium [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] class with Statistics, explicit equations and Numerical T_C Predictions. Residuals and errors for the ILS MEM are studied and statistical graphics with 97% Confidence intervals are shown. The MATLAB MEM 2D shapes ratifie clearly sinusoid MEM curves got in [43, 44]. Electronics Physics applications emerge from all the results.

Mathematical and computational methods

The MEM MATLAB computational method experimental data and implemented algorithm is developed almost equal in

equations than the ones presented in [1, 4-6, 42, 43, 44]. However, this research covers T_C data for [$T_C < 0°$, $T_C > 0°$]. Software is developed in MATLAB with subroutines and patterns improved to obtain numerical data such as original Tables 3-6. Optimization algorithm is constructed with Inverse Tikhonov Regularization Theory [7, 13, 31, 42, 43, 44]. Table 1 shows Numerical Experimental Data for MEM [4-6, 12-15, 32-34, 37, 42, 43, 44]. Table 2 widens T_C data for [$T_C < 0°$], but Tetragonal Lattice and Amorphous compounds are not included yet.

Table 1: The development data [$T_C > 0°$] for optimization of parameters for Graphical/Numerical-Algorithms MEM in Thallium HTSCs [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] class implemented like in [43, 44]. This method was used in previous studies with different HTSCs materials [1, 42, 43, 44].

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: The development data [$T_C < 0°$] for 2D Graphical and Numerical Optimization of MEM parameters in HTSCs [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Thallium group implemented [1, 42, 43, 44].

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

Basic MEM formulas/algorithms from [4-6, 12-15, 32-34, 37, 42, 43, 44] are implemented in MATLAB for this study. Equation (1) shows Inverse Tikhonov functional method like [42, 43, 44]. The formulation algorithm of Isotope Effect comes from [1, 42, 43, 44]. The ILS Inverse Tikhonov algorithm MEM, with a polynomial p(MO) reads,

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

(1)

where, as [1, 4-6, 42, 43, 44], MO is the molecular mass of the HTSC selected (i) within a HTSC group with (i) elements and [a-b] are constraints intervals. T_{Ci} is every critical temperature (Centigrade in this MEM Thallium HTSCs class) for each (i) member of HTSCs group. The figure α1 is a specific constant for Inverse Tikhonov Regularization. The constraints, related to T_C and MO values from experimental data, [a-b], are implemented in optimization. Linear Logarithmic-form, like in Equation (1) of [44], could also be used.

Results

First results section is 2D MEM Graphical Statistical-Optimization of MEM Thallium class for [$T_C < 0°$, $T_C > 0°$], Fig 1, 2. Those graphs confirm MATLAB and GNU-Octave solutions obtained in [43, 44]. Second section shows ILS Numerical Equations for 4, 5 polynomial-degrees, Tables 3, 4, and respectively their Numerical Prediction, Tables 5, 6. Optimal ILS MEM numerical results correspond to Tables 3, 4. In Tables 3,4, it is proven the 4, 5-degree finest MEM [42, 43, 44]. Fig 3 from [44], shows a GNU-Octave dual-optimization for Thallium class constrained to [$T_C > 0°$], which validates the analytic geometry of Statistical Fig 1, 2. Definitely, MEM sinusoid-like shape is demonstrated for this Thallium HTSCs group, in contrast with parabolic curves for MEM of [Sn-Sb-Te-Ba-Mn-Cu-O] class [42].

2D Statistical Optimization

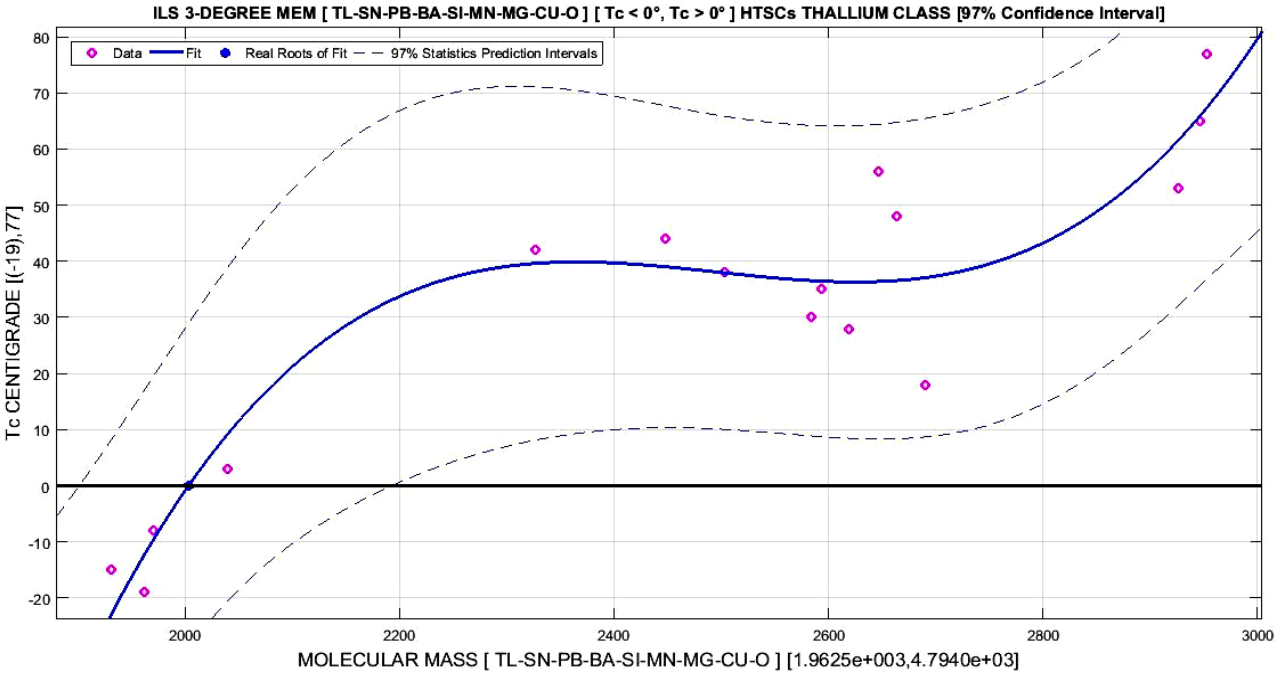

Fig 1: - 3-Degree Matlab polynomial MEM 2D Graphical Statistical Optimization with 97% Confidence Interval for MEM [$T_C < 0°$, $T_C > 0°$]. Experimental data [red points], MEM curve [blue], Confidence Intervals [dashed-blue lines]. Running time is approximately 2-5 seconds shorter than GNU-Octave [44].

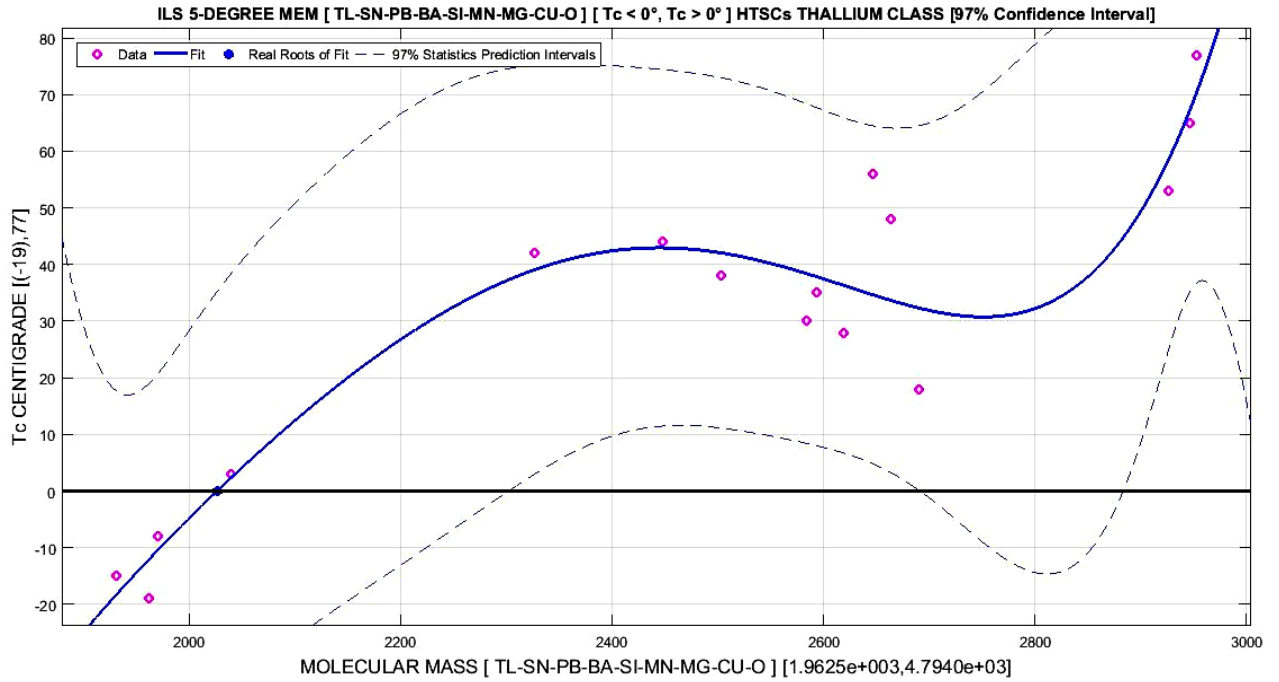

Fig 2: - 5-Degree Matlab polynomial MEM 2D Graphical Statistical Optimization with 97% Confidence Interval for MEM [$T_C < 0°$, $T_C > 0°$]. Experimental data [red points], MEM curve [blue], Confidence Intervals [dashed-blue lines]. Running time is approximately 2-5 seconds shorter than GNU-Octave [44].

Numerical Equations for [$T_C < 0°$, $T_C > 0°$] and T_C Predictions

The numerical ILS polynomial explicit equations are shown in Tables 3,4. T_C Predictions for 4- and 5-degrees ILS polynomial fits are presented at Tables 5,6. Residuals are acceptable, although errors are rather high about [+/- 6 Centigrade]. Fig 3 from [43], shows a comparative previous GNU-Octave dual-optimization for Thallium class constrained to [$T_C > 0°$], which confirms the analytic geometry of Fig 1, 2.

Table 3: MATLAB software 4-degree ILS MEM polynomial equation Thallium HTSCs class [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group subject to [$T_C < 0°$, $T_C > 0°$]. 4th coefficient is discarded [$\approx 10^{-12}$]. Residual magnitude is acceptable.

ILS MEM (4-DEGREE) [$T_C < 0°$, $T_C > 0°$] WITH APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
18.2941e+003	CONSTANT
-33.2825	X
22.2890e-003	X^2
-6.5225e-006	X^3
≈ 0	X^4
RESIDUAL = 5.8733	
MODEL EQUATION	
Tc = [18.2941e+003] +… … + [-33.2825] MO + … … +[22.2890e-003] MO^2 +… …+ [-6.5225e-006] MO^3	

Table 4: Matlab software 5-degree ILS MEM polynomial equation Thallium HTSCs class [Tl- Sn-Pb-Ba-Si-Mn-Mg-Cu-O] HTSCs group subject to [$T_C < 0°$, $T_C > 0°$]. 5th coefficient is discarded [$\approx 10^{-12}$]. Residual magnitude is acceptable. Curve graphics corresponds to Fig 2.

ILS MEM (5-DEGREE) [$T_C < 0°$, $T_C > 0°$] WITH APPROXIMATIONS	
COEFFICIENT	VARIABLE X SELECTED
-36.6798e+003	CONSTANT
83.1217	X
-75.7464e-003	X^2
34.5266e-006	X^3
-7.8399e-009	X^4
≈ 0	X^5
RESIDUAL = 5.8627	
MODEL EQUATION	
Tc = [-36.6798e+003] +… … + [83.1217] MO + … … +[-75.7464e-003] MO^2 +… …+ [34.5266e-006] MO^3 +… …[-7.8399e-009] MO^4	

Table 5: - 4 Degree ILS MEM MATLAB Numerical Predictions, [MO Molecular Mass, T_C Experimental, T_C MEM Predicted, Error ([T_C Experimental] - [T_C Predicted])]. Error magnitude probably is caused by the nonlinear increase of Molecular Mass related to increment of T_C [43, 44].

OPTIMIZATION PREDICTIONS Tc MEM ILS 4-DEGREE FOR [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O]

MO	Tcexperimental	TcPredicted	Error
1962.4934	-19	-12.29724416104	-6.70275583896
1930.9474	-15	-17.4814367218241	2.48143672182414
1970.1884	-8	-10.9672729743106	2.96727297431062
2040.0584	3	1.72313682971071	1.27686317028929
2690.7295	18	33.1603583123251	-15.1603583123251
2619.4897	28	35.9129062684005	-7.91290626840055
2583.8698	30	37.725694948087	-7.72569494808704
2593.32105	35	37.2374662029069	-2.23746620290694
2503.4204	38	41.467505094035	-3.467505094035
2326.4404	42	40.5461494010051	1.4538505989949
2447.9369	44	42.9321709180404	1.06782908195964
2663.6085	48	33.9826050291704	14.0173949708296
2926.2966	53	59.8710061720994	-6.87100617209944
2646.15	56	34.6788220733288	21.3211779266712
2946.0781	65	66.873193420648	-1.87319342064802
2953.1491	77	69.634939187592	7.36506081240805

Tc PREDICTED ERROR [Average Error 6.4939]

Table 6: - 5 Degree ILS MEM MATLAB Numerical Predictions, [MO Molecular Mass, T_C Experimental, T_C MEM Predicted, Error ([T_C Experimental] - [T_C Predicted])]. Error magnitude probably is caused by the nonlinear increase of Molecular Mass related to increment of T_C [43, 44].

OPTIMIZATION PREDICTIONS Tc MEM ILS 5-DEGREE FOR [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O]

MO	Tcexperimental	TcPredicted	Error
1962.4934	-19	-12.0112767767278	-6.98872322327225
1930.9474	-15	-18.3798003591728	3.3798003591728
1970.1884	-8	-10.5068799347937	2.50687993479369
2040.0584	3	2.38526592669223	0.614734073307773
2690.7295	18	32.2942191204929	-14.2942191204929
2619.4897	28	36.2856249362594	-8.28562493625941
2583.8698	30	38.4045517514314	-8.40455175143143
2593.32105	35	37.8572058827194	-2.85720588271943
2503.4204	38	42.0434893506099	-4.04348935060989
2326.4404	42	39.0515845606642	2.9484154393358
2447.9369	44	42.9475051509144	1.05249484908563
2663.6085	48	33.6745335091582	14.3254664008418
2926.2966	53	58.5595172907779	-5.55951729077788
2646.15	56	34.6774238307917	21.3225761692083
2946.0781	65	67.1338437244558	-2.13384372445581
2953.1491	77	70.5831919489792	6.41680805102078

Tc PREDICTED ERROR [Average Error 6.5709]

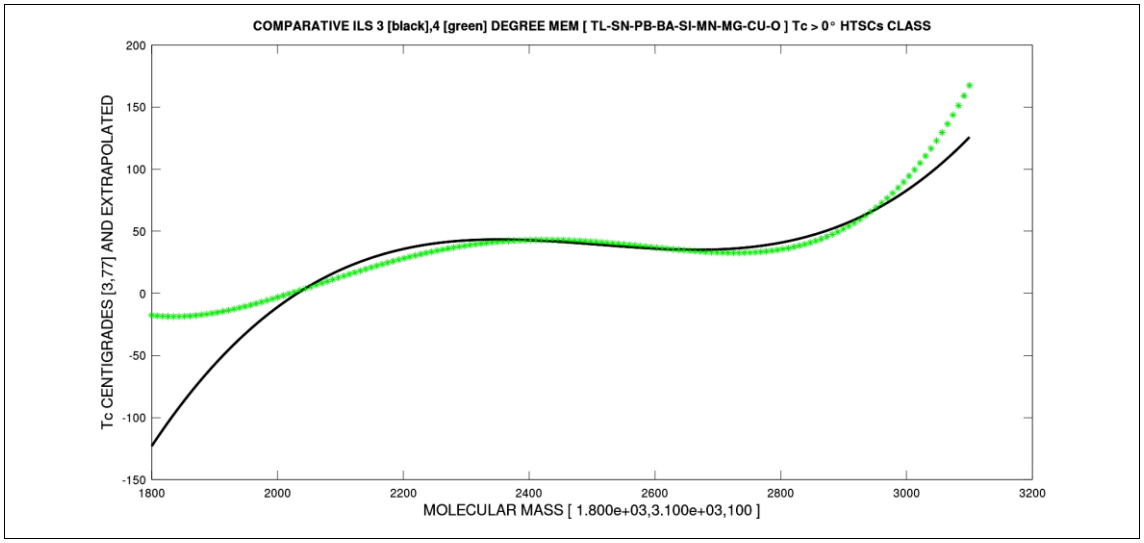

Fig 3: - From [44], an illustrative 3-4 Degree comparative dual-approach, GNU-Octave, with 3, 4-Degree ILS MEM polynomial optimization for [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] Thallium HTSCs group. 3-Degree (black) is linear, and it is seen how when passing on 4-Degree (green) polynomial the curve begins to take sinusoid shape. Overlap is almost complete along the experimental data line, which proves the fit correctness. Experimental MEM data is not implemented as it would create an unclear image. Since this HTSCs class has a number of compounds with $T_C < 0°$, MEM confirms clearly that affinity with the green 3, 4-Degree shape [43, 44].

Discussion and conclusions

The objective of this continuing research was to broaden the HTSCs Thallium class T_C range, implementing more experimental database from $T_C < 0°$ to improve previous studies [42, 43, 44]. There are three strands, numerical determination of new ILS MEM equations, 2D Statistical-Graphical Optimization to validate the analytical geometry of the Thallium class MEM, and numerical predictions of T_C based on these data.

The curves obtained confirm the shapes obtained in previous research [43, 44] for $T_C > 0°$ exclusively [43, 44]. ILS polynomial equations result very similar numerically than [43, 44]. Predictions errors are about [+/- 6], and this figure can be considered rather too high at this MEM stage.

The reasons for these prediction errors could be the nonlinear increase of the T_C values related to molecular mass, Tables 1, 2. However, tetragonal compounds of this group were not included into implemented data for ILS MEM optimization.

MATLAB 2D Graphical Optimization validates results got with GNU-Octave in [44]. MATLAB imaging processing running time is shorter than GNU-Octave [44], about 2-5 seconds, and imaging quality is approximately equal.

In brief, this MEM following study broadens imaging and numerical data with the inclusion of [$T_C < 0°$] data. It has improved and provided/confirmed previous results [43, 44]. However, MEM numerical predictions errors are rather high at this stage. Applications in Electronics Physics of HTSCs Thallium class could be obtained from 2D Numerical/Graphical and Numerical Predictions analysis results.

Scientific ethics standards

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]. This article comprises original GNU-Octave software-variation related to previous publications series [1, 4-6, 42, 43]. 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 GNU-Octave constitutes a software engineering improvement from previous contributions [1, 4-6, 42, 43]. 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, 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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