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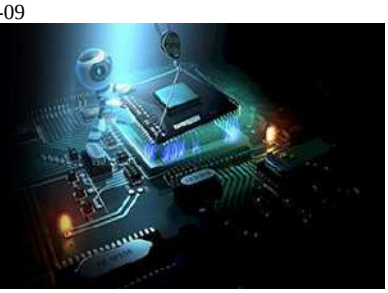

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# Genetic algorithms molecular effect model optimization computational method for high temperature superconductors

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**Abstract**
Genetic algorithms software was applied in 3D Graphical and Interior Optimization methods for two High Temperature Superconductors (HTSCs) classes. Namely, Tin (Sn) class with [$T_C > 0°$] and Thallium ($T_l$) one subject to [$T_C < 0°$, $T_C > 0°$] in Molecular Effect Model (MEM). Results comprise Tikhonov Regularization Functional mathematical algorithms for these HTSCs group without using logarithmic changes. Results also show the contrasts between these two classes for Molecular Effect Model (MEM) hypothesis. Solutions show a series of 2D/3D imaging process charts complemented with a group of numerical results. Electronics Physics applications for Superconductors and High Temperature Superconductors and Medical Technology are specified for MEM and presented.

**Keywords:** Genetic Algorithms (GA), Molecular Effect Model (MEM), Interior Optimization (IO), Graphical Optimization (GO), Systems of Nonlinear Equations, Critical Temperature ($T_C$). Tikhonov Regularization (TR), Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory, [Sn-Sb-Te-Ba-Mn-Cu-O] Tin Molecular HTSC Group, [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O], Thallium Molecular HTSC Group Molecular Mass (MO), BCS Theory

## Introduction
Previously, Dual Least-Squares combined with Genetic Algorithms (GA) method was applied on Hg-Cuprates and Tin (Sn) group HTSC class [3-5, 48, 49, 50] with primary acceptable results [49, 50]. This method is extended here to Thallium (Tl) class subject to [$T_C < 0°$, $T_C > 0°$] in Molecular Effect Model (MEM). GA methods have proven be efficient in optimization and large-scale optimization in several branches of applied science and engineering [3-9, 48-50]. Dual-optimization methods with two algorithm types [50], Inverse Least Squares and GA, provided 2D/3D simulations with theoretical/experimental results from the literature [3-6, 39m, 48, 50] were published in former contributions.
When differences of molecular weightt due to proportion/isotopic-variation in the HTSC molecule occur, the Molecular Effect mathematical model to approximate/predict the $T_C$ magnitude changes for every HTSC group compounds may be useful/efficacious. Both classical Isotope Effect and MEM could be useful for $T_C$ prediction equations in Superconductors and HTSCs. However, Isotope Effect is experimentally established within BCS theory, while MEM is a hypothetical method at present [48-50].
Therefore, the improvements of this research are given by the original software for GA methods in these HTSCs classes. Innovation consists to set at Z axis the absolute difference between MEM $T_C$ and experimental $T_C$. The programming is used to study the proper characteristics of each HTSCs class programmed with 2D-GA and 3D Graphical Optimization methods [3-5, 48-50].
The software method applied in this study is set with GA Matlab tools. In [50], a dual method ILS-GA was implemented for HTSC Tin (Sn) class. The first program, at [50], was a 2D polynomial fit to obtain approximate polynomial coefficients boundaries and confirm the MEM analytic geometry shape. Then, with this data the refinement and confirmation of the numerical results are got through a GA second program. The main advantage of this method was make sure of the numerical results cogency.
Results of this research comprise GA MEM for Tin and Thallium HTSCs classes. 2D/3D GA Graphics of program performance, and final $T_C$ polynomial predictive equations. The

novelty of this study is the GA application following results got in previous contributions [3-5, 48, 49]. In brief, the article shows a 2D/3D Graphical Genetic Algorithm Optimization study for the primary hypothesis of MEM for Tin and Thallium HTSCs classes. Algorithms are implemented with Matlab software and 2D/3D Graphical MEM model imaging processing methods.

## Mathematical and Computational Method

Tables 1-3 show the software programming implementation data for Equation (1) the programming algorithm implemented [3-5, 48-50]. The Tikhonov Functional is improved from previous research [49, 50], Equation 1. The difference with other former studies is the setting of MEM algorithm objective function at Z axis in Figures 2-3, and 5-7. The dataset was applied in multifunctional charts into GA program, Figures 1 and 4. First stage method comprises the GA polynomial fit to obtain multifunctional graphics. Second stage is implement GA results into 3D Graphical optimization charts. With GA program, the refinements to obtain the MEM optimal fitness sectors are got. The previous program method Flow Chart is explained in [49, 50].

**Table 1:** The development of optimization of parameters for [Sn-Sb-Te-Ba-Mn-Cu-O] group implemented in this study [1, 3-5, 12-15, 48-50]. This table is taken from [1, 3-5, 12-15, 48-50] as the numerical initial data is the same for different mathematical-computational task

| Numerical Optimization Data For Sn-Sb-Te-Ba- Mn-Cu-O Group [HT-Superconductor, Molecular Effect hypothesis] | |
|---|---|
| **Formulation** | **Molecular Weight (UAM) / Approximate To(Kelvin)** |
| Sn10SbTe9Ba2MnCu21O42+ | 4.7940e+003/+187 C |
| Sn9SbTe8Ba2MnCu19038+ | 4.3565e+003/+187 C |
| Sn8SbTe7Ba2MnCu17O34+ | 3.9190e+003/+167 C |
| Sn7SbTe6Ba2MnCu15030+ | 3.4816e+003/+155 C |
| Sn10SbTe4Ba2MnCu16O32+ | 3.6778e+003/+141 C |
| Sn9SbTe4Ba2MnCu15030+ | 3.4635e+003/+136 C |
| Sn8SbTe4Ba2MnCu14O28+ | 3.2493e+003/+129 C |
| Sn9SbTe3Ba2MnCu14O28+ | 3.2403e+003/+121 C |

**Table 2:** The development of optimization of parameters for Thallium Molecular HTSC Group, [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] implemented in this study [1, 3-5, 12-15, 48-50] at [$T_C > 0$ °C]. This table is taken from previous papers database [1, 3-5, 48, 49, 50] because the numerical initial data is the same for different mathematical-computational task

| Numerical Optimization Data [TI-Sn-Pb-Ba-Si-Mn-Mg-Cu-O) Class [HT-Superconductors, [Tc > 0°] Molecular Effect Hypothesis | |
|---|---|
| **Formulation** | **Molecular Weight (UAM) / Approximate Tc (Centigrades)** |
| T17Sn2Ba2MnCu10020 | 2.9531e+03 /77 |
| T17Sn2Ba2TiCu10020 | 2.9461e+03 |
| T16Sn2Ba2TiCu9018 | 2.6462e+03 |
| T17Sn2Ba2SiCul0020 | 2.9263e+03/5 |
| T16Ba4SiCu9O18 | 2.6636e+03/49 |
| TI5Ba4SiCu8O16 | 2.4479e+03 |
| (TISSn2) Ba2SiCu8O16 | 2.3264e+03 |
| (TISPb2) Ba2SiCu8O16 | 2.5034e+03 |
| (TI5Pb2) Ba2Si2.5Cu8.5017 | 2.5933e+03/3 |
| (T15Pb2) Ba2Mg2.5Cu8.5017 | 2.5839e+03/3 |
| (TI5Pb2)Ba2Mg2Cu9O18 | 2.6195e+03/28 |
| (TI5Pb2) Ba2MgCu10O20 | 2.6907e+03/ |
| (T14Pb) Ba2MgCu8O13 | 2.0401e+03 |

**Table 3:** The development of optimization of parameters for Thallium Molecular HTSC Group, [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] implemented in this study [1, 3-5, 12-15, 48-50] at [$T_C < 0$ °C]. This table is taken from previous papers database [1, 3-5, 48, 49, 50] because the numerical initial data is the same for different mathematical-computational task

| Numerical Optimization Data [TI-Sn-Pb-Ba-Si-Mn-Mg-Cu-O) Class [HT-Superconductors, [Tc < 0°] Molecular Effect Hypothesis | |
|---|---|
| **Formulation** | **Molecular Weight (UAM) / Approximate Tc (Centigrades)** |
| (T14Ba) Ba2MgCu8O13 | 1.9702e+003 /-8 |
| (TI4Ba) Ba2Mg2Cu7O13 | 1.9309e+003/-15 |
| (T14Ba) Ba2Ca2Cu7013 | 1.9625e+003/-19 |

For this Molecular Model, the constraints values for parameters are shown in Tables 1-3. The algorithms set for GA Molecular Effect, with a polynomial P ($MO_i$ ) read.

$$
\begin{aligned}
&\text{minimize Tikhonov functional } J(\alpha), \\
&\text{with } \alpha 1 = 0 \text{ and } L_2 \text{ Norm}, \\
&J_{\alpha}(u)_{u \in R} = |A\,u - MO|_1 + [\alpha 1]\, J(u); \\
&\text{Hence minimize Chebyshev Norm}, \\
&|T_{Ci} - p(MO_i)|_1, \\
&\text{for } i = 1, \ldots\ldots n \\
&\text{subject to}, \\
&a \le MO_i \le a_1; \\
&b \le T_{Ci} \le b_1;
\end{aligned}
\tag{1}
$$

Where
$J_{\alpha}(u)$: Functional with regularization parameter alpha.
R: Real space.
U: Searched parameter solution.
$MO_i$: Molecular mass for HTSC Sn and Tl HTSCs classes. Tables 1-3.
$P(MO_i)$: Polynomial optimization parameter matrix. HTSC Sn and Tl ranges Tables 1-3.
A1: Constant parameter. Tikhonov Regularization Parameter, selected null.
| • |: $L_1$ Chevyshev Norm (at algorithm software absolute value).
A, $A_1$: Constraints range specified at Tables 1-3 for HTSCs Sn and Tl classes.
B, $B_1$: Constraints range specified at Tables 1-3 for HTSCs Sn and Tl classes.

## GA Programming Method

The programming basis are related to previous contributions [3-5, 48, 49, 50] and dual-program design [50]. In software and imaging processing details with explanations are set. All programming was developed from these articles series to form the base of this new one.

## Results

The results are divided into two parts. First one is Tin 2D/3D Graphical Optimization results, Figures 1-3. Second part corresponds to Thallium 2D/3D imaging charts, Figures 4-7. Figures 1 and 4 show the Genetic Algorithms software results with imaging processing multifunctional graphics. A brief of numerical results for both HTSCs classes is included in Table 4.

**2D/3D Results Sn GA Optimization**

Figure 1 shows the 2D GA polynomial model in a multifunctional chart like in [49, 50]. Figure 2 presents the optimal model sector for this MEM. The optimal zones for model are marked inset with arrows. Figure 3 represents MEM Tin HTSCs model in simple grayscale. This parabolic analytic geometry for Tin class was obtained in previous research with ILS method [3-5, 48, 49, 50], Figures 2-3. The Thallium class show a sigmoidal analytic geometry, [3-5, 48-50] and references in those papers]. Figures 1 and 4 prove the GA program performance in a multifunctional chart. The most important parts are the Best fit that gives the fitness value, and the percentage of criteria met. The other parts show complementary information, such as best, worst and mean scores, stopping criteria and children number evolution. This type of software was initially developed in [48, 49, 50].

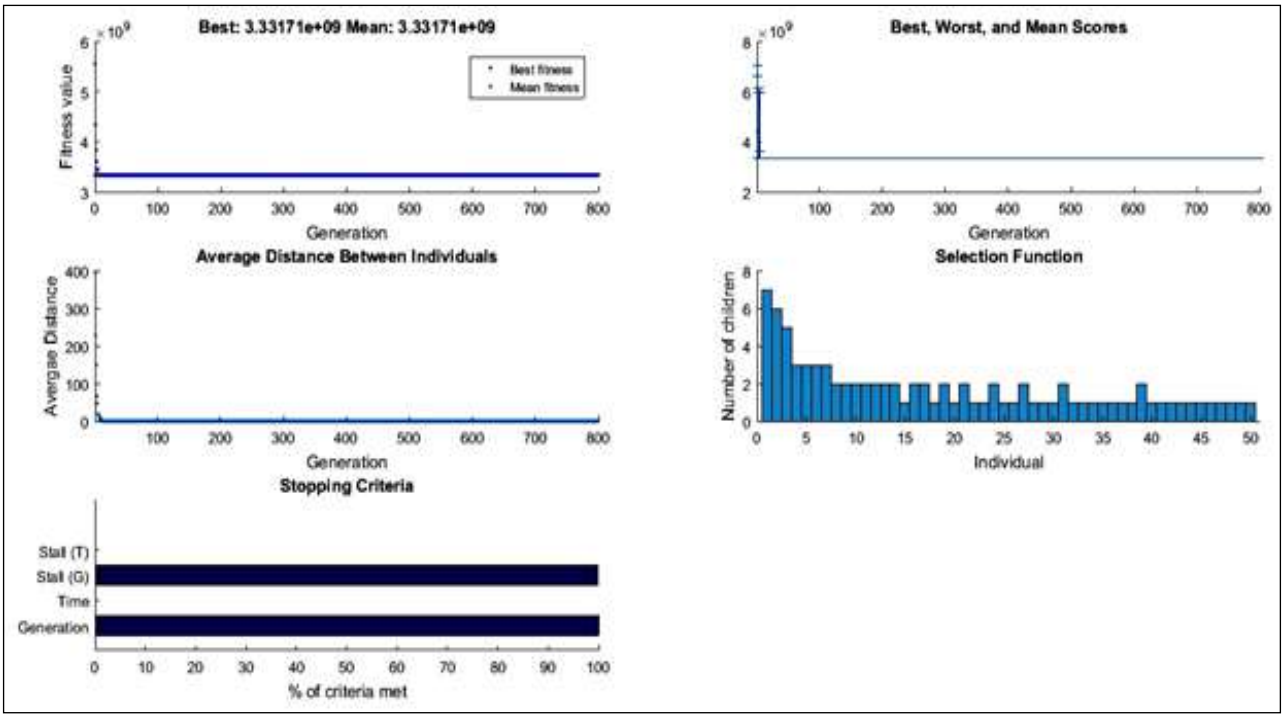


**Fig 1:** The GA programming multifunctional 2D graph. 2D Sn polynomial fit parameters intervals set into GA program with Matlab. Generations Number is 800. As it was found in previous contributions, for Sn class the MEM shows in [50] an approximate 2D parabolic shape [3-5, 48, 49, 50]

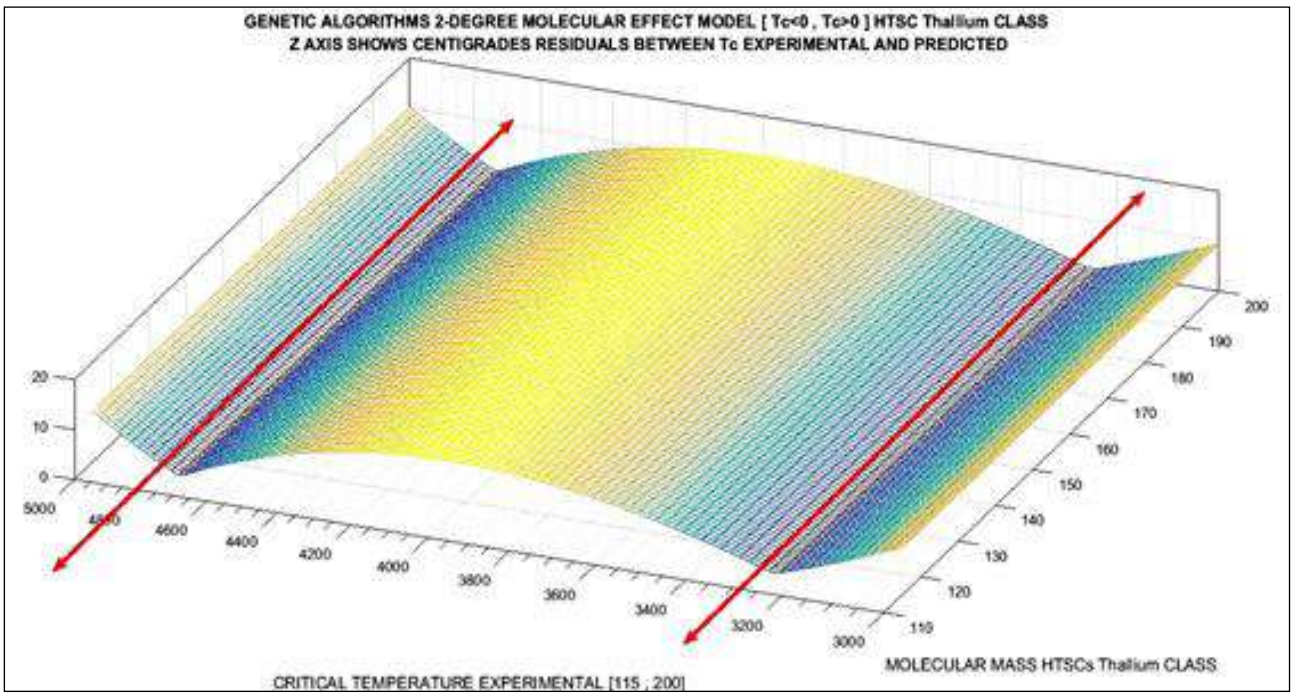


**Fig 2:** Optimal MEM sector for Tin HTSC class. It was set as in [50] a 2-Degree polynomial MEM model. 2D polynomial fit parameters intervals were obtained from GA program with Matlab. Generations Number is 500-800 for getting these polynomial coefficients. As it was found in previous contributions, for Sn class the MEM shows get an approximate 2D parabolic shape [3-5, 48, 49, 50]. Model fits approximately well between molecular weights interval [3200, 4700] for all values of $T_C$

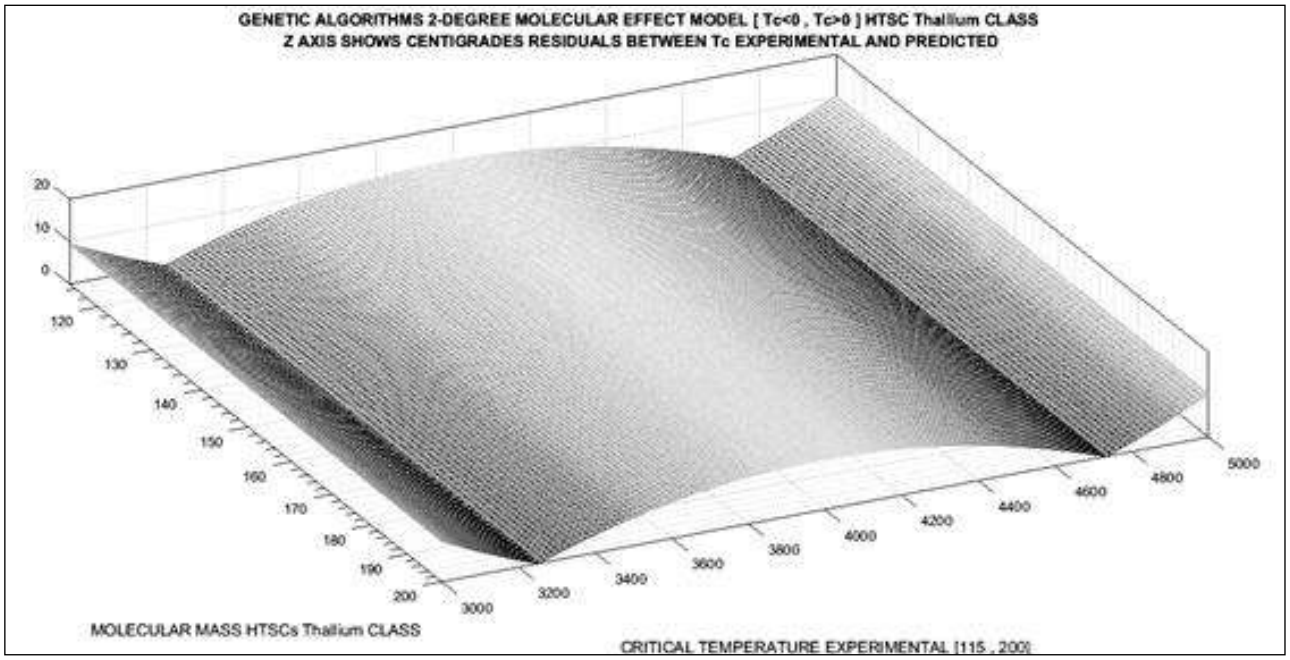


**Fig 3:** Grayscale imaging processing for Optimal MEM sector for Tin HTSC class. It was set as in previous study, [50], a 2-Degree polynomial MEM model. 2D polynomial fit parameters intervals were obtained from GA program with Matlab. Generations Number is 500-800 for getting these polynomial coefficients. As it was found in previous contributions, for Tin (Sn) class the MEM shows get an approximate 2D parabolic shape [3-5, 48, 49, 50]. Model fits approximately well between molecular weights interval [3200, 4700] for all values of $T_C$

## 2D/3D Results Thallium (Tl) class with best-fitness in 3th Degree Polynomial

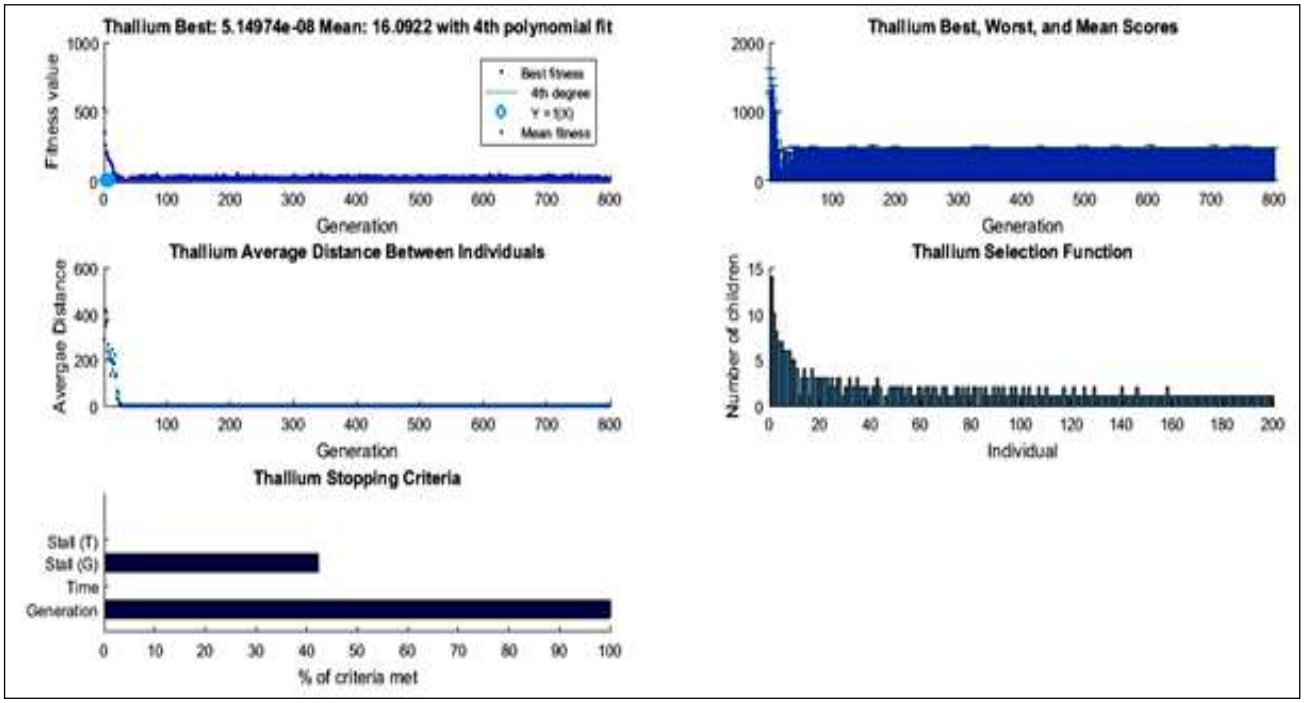


**Fig 4:** The Thallium HTSCs class GA programming multifunctional 2D graph, 2D Tl polynomial fit parameters

Intervals set into GA program with Matlab. Generations Number is 800. Best fit with 3-Degrees polynomial line, Table 4, inset first graph. As it was found in previous contributions, for Tl class the MEM shows in [50] an approximate 2D sigmoidal analytic geometry shape [3-5, 48, 49, 50]

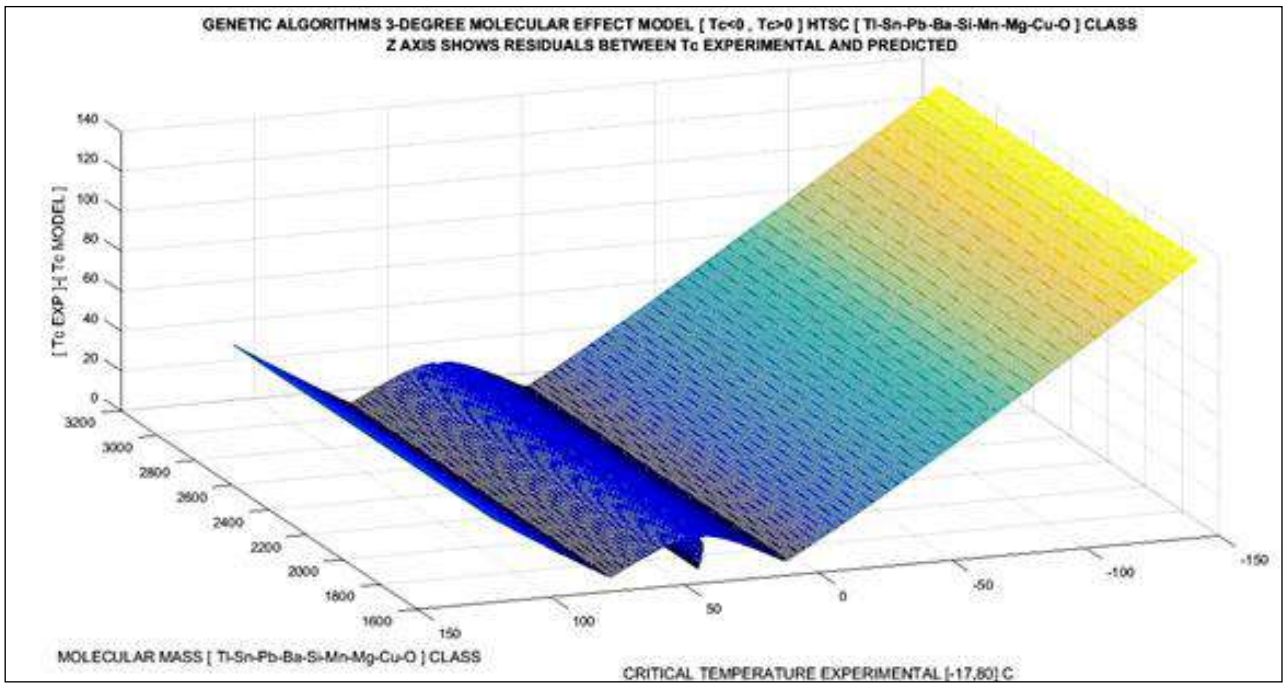


**Fig 5:** Optimal MEM sector for Thallium HTSC class. It was set as in [48, 49, 50] a 3-Degree polynomial MEM model. 2D polynomial fit parameters intervals were obtained from GA program with Matlab in Figure 4. Generations Number is 500-800 for getting these polynomial coefficients. As it was found in previous contributions, for Tl class the MEM shows get an approximate 2D sigmoidal shape [3-5, 48-50]. Model fits approximately well between MEM temperatures interval [0, 75] Centigrades for all values of Molecular Mass

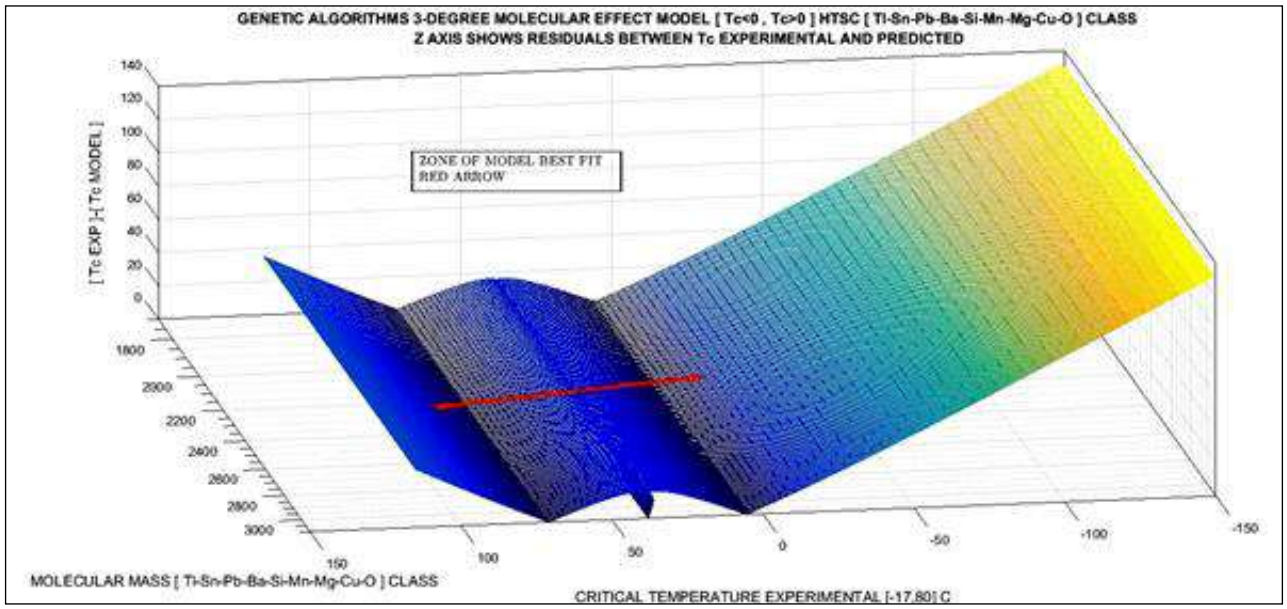


**Fig 6:** Other image processing perspective with optimal sector marked inset. Optimal MEM sector for Thallium HTSC class is approximately wide. It was set as in [48, 49, 50] a 3-Degree polynomial MEM model. 2D polynomial fit parameters intervals were obtained from GA program with Matlab in Figure 4. Generations Number is 500-800 for getting these polynomial coefficients. As it was found in previous contributions, for Tl class the MEM shows get an approximate 2D sigmoidal shape [3-5, 48-50]. Model fits approximately well between MEM temperatures interval [0, 75] Centigrades for all values of Molecular Mass

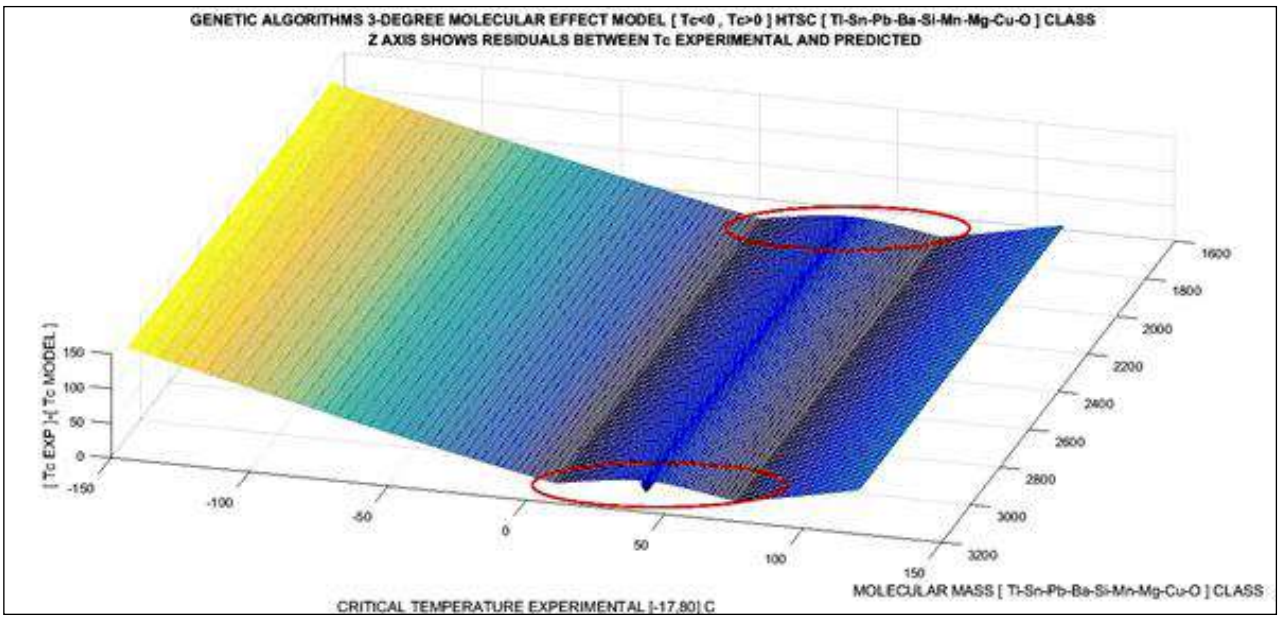


**Fig 7:** Other image processing perspective with optimal sector elliptic-marks inset. Optimal MEM sector for Thallium HTSC class is approximately wide. It was set as in [48, 49, 50] a 3-Degree polynomial MEM model. 2D polynomial fit parameters intervals were obtained from GA program with Matlab in Figure 4. Generations Number is 500-800 for getting these polynomial coefficients. As it was found in previous contributions, for Tl class the MEM shows get an approximate 2D sigmoidal shape [3-5, 48, 49, 50]. Model fits approximately well between MEM temperatures interval [0, 75] Centigrade for all values of Molecular Mass.

## Brief Numerical Results for HTSCs Sn and Tl Classes

Table 4 shows all the dual numerical results with errors for both HTSCs classes. Errors can be considered acceptable. Note the 500-800 number of GA generations

**Table 4:** Brief of Numerical results for both HTSCs classes MEM optimization (polynomial) in 2D/3D Graphical GA implementation of software. For Sn class, error is higher in GA because for GA the program was done for 800 generations, and for polynomial fit was made for 200 functions. For Thallium class residual can be considered acceptable

| **Brief of numerical results Method** | | |
|---|---|---|
| **Tin (SN) HTSCs Class** | | |
| **Stage** | **Method** | **Comments** |
| **First** | Genetic Algorithm Tikhonov Functional | Program and 2D graphics patterns [Figure 1] |
| **Second** | Implementation Into 3D Graphical optimization charts. | Program and Multigraphics pattern [Figures 2-3] |
| **Optimal MEM Sector** | | |
| Between molecular weights interval [3200, 4700] for all values of Tc | | |
| **Polynomial MEM Equation** | | |
| Tc =[-21.7822e-006] MO2+[216.4114e-003] MO+[-347.6922] | | ERROR [200 functions] 4.5173e+000 |
| **Genetic Algorithm MEM Equation** | | |
| Tc = [ -20.7821e-006] MO2+ [217.4114e-003] MO ++[ -346.6922 ] | | ERROR [500-800 generations 57.7211e+003 |
| **Thallium (TI) HTSCs Class** | | |
| **Best GA fit Equation** | | **Polynomial Degree and Norm of residuals** |
| y=p1*x^3+p2*x^2+<br>p3*x + p4<br>Coefficients:<br>p1 = -5.9232e-09<br>p2 = 8.1346e-06<br>p3 = -0.00326<br>p4 = 0.34885 | | Degree: 3<br>Norm of residuals =<br>10.372 |
| **Optimal MEM Sector** | | |
| MEM Optimal Tc sector interval [0, 75 ] Centigrades for all values of Molecular Mass<br>Program and Multigraphics patterns [Figures 4-7] | | |

## Applications

Table 5 improved form [48, 49, 50] shows overview of applications for MEM one. Molecular Effect applications are guessed and developed from experimental literature database [3-5, 39-50]. Applications are at this stage theoretically deduced [3-5, 14, 15, 28, 39-50]. MEM usages were also detailed in previous contributions [48-50]

**Table 5:** Improved from [48-50], brief of applications for the MEM that were explained in former contribution series [3-5, 48-50].

| Superconducting Molecular Effect Primary Applications | | |
|---|---|---|
| **Type** | **Use** | **Additional** |
| General 2D Tc / Molecular Mass curve shape, Parabolic for Sn class Sigmoidal for TI class | For catching up the approximate variation of Tc related to Molecular Mass. This is useful for guess of possibility of Tc predictions | Every HTSC class shows get a proper 2D shape. Usually parabolic inverse, but sigmoid can occur also [Thallium class, 3-8,39-48-50] |
| When there are several isotopes types in different proportions in the sample that cause variations in Molecular Mass | Approximations/predictions for Tc could be got from the 2D curve equations and 3D Graphical Optimization | Approximations to be confirmed by experimental dataset |
| When there are several isotopes types in different valences in the sample that cause a different Molecule within the HTSC class | Approximations/predictions for Tc could be got from the 2D curve equation | Approximations to be confirmed by following experimental data |
| When both phenomena happen. Different valences, and isotopes proportions in the prospective HTSCs experimental work | Approximations/predictions for Tc could be got from the 2D curve equation | Both theoretical and experimental task |
| Inverse Optimization of isotopes in molecule proportion to obtain a desirable Tc | Precision to reach a desired or optimal Tc | Theoretical approach |

## Discussion and Conclusions

This research objective was to prove/show the Genetic Algorithm Dual-Polynomial Optimization method for prediction results for MEM in Tin HTSCs class, subject to [$T_C > 0°$], Table 1, and Thallium one, tables 2-3, for [$T_C < 0°$, $T_C > 0°$]. The novelty of this study is the GA application following results got in previous contributions [3-5, 48-50]. In these HTSCs groups, MEM model was 2D/3D graphically optimized, with polynomial-fitness, and numerically studied with GA Equation (1). Multifunctional GA software 2D graphics were obtained, Figures 1 and 4.

Results 2D/3D MEM polynomial Objective Function Graphical and Numerical Optimization database. 3D imaging processing proves the Tin class approximately parabolic-shaped curvatures and numerical-graphical extrapolations for $T_C$. In Thallium class, MEM optimal sectors were got in Figures 5-7. Numerical results for both HTSCs groups are approximately acceptable, Table 4. These HTSC groups MEM [Casesnoves, 2020], 2D analytical geometry shapes and 3D MEM Objective Functions curvatures can be considered approximately satisfactory with low residuals, Table 4, Figures 1-7. A number of applications for MEM are detailed, Table 5.

Advantages of this GA software method are the 2D/3D improved mathematical and geometrical numerical analysis for the MEM optimization. Inconvenients with GA programming multifunctional 2D imaging processing was the increasing running time, about 2-4 minutes, when several GA optimization parameters and numerical statistics are implemented in a unique graph. The higher number of generations, the longer running gradient time in GA compared to other optimization Inverse Least Squares techniques used previously [3-6, 39, 48-50].

Software methods and programming was based on previous contributions [3-9, 48-50]. GA specific patters for every graph and numerical predictions were improved from [49, 50]. The programming for Figures 1 and 4 requires arranging of GA special commands, patterns, loops, optimal running time choice, and setting precise upper and lower boundary limits for constraints.

*Grosso modo*, a 2D/3D GA methods for MEM subject to Tin and Thallium HTSCs classes have been presented for MEM. Applications in Electronics/Electromagnetics and Materials Physics emerge from the study results, Table 5.

## Scientific ethics standards

2D/3D Graphical Optimization Methods were created by Dr Francisco Casesnoves in 3rd November 2016, and Interior Optimization Methods in 2019. 4D Graphical and Interior Optimization Methods were created by Dr. Francisco Casesnoves in 2020. MEM was firstly developed by author in 15th March 2021. This GA new software was originally developed by author. This article has previous papers information, whose inclusion is essential to make the contribution understandable. Table 5 is improved/adapted from [50]. The GA nonlinear optimization software was invented/improved from previous contributions in subroutines modifications, patters, loops, graphics and optimal visualization [49, 50]. At Method section, algorithm for basic Tikhonov Functional was developed from [3-5, 48-50]. The 4D Interior Optimization method is original from the author (August 2021). This study was carried out, and their contents are done according to the European Union Technology and Science Ethics and International Scientific Community Ethics [37, 38]. 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 citation such as [Casesnoves, 'year'] appears, there is not vanity or intention to brag. The reason is to set clearly, at present research times, the intellectual property. When a mathematical statement, proposition or theorem is presented, demonstration is always included if it was not set in previous papers. When 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 [37, 38].

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