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EVOLUTIONARY ALGORITHMS MOLECULAR EFFECT MODEL OPTIMIZATION FOR HIGH TEMPERATURE SUPERCONDUCTORS CUPRATES AND REVIEW OF TIN AND THALLIUM CLASSES

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ABSTRACT

Genetic Algorithms (GA) Artificial Intelligence (AI) software was applied in 3D Graphical and Interior Optimization methods for several High Temperature Superconductors (HTSCs) classes. Namely, Hg-Cuprates HTSCs, [Hg-Ba-Ca-Cu-O] with [$TC > 0^{\circ}$], and a extent review for Tin (Sn) class with $\lceil TC \rceil$ and Thallium (Tl) one subject to $\lceil TC \rceil$ $\lceil TC \rceil$, $\lceil TC \rceil$ in Molecular Effect Model (MEM). Results comprise both improvements and evaluation with Tikhonov Regularization Functionals algorithms for these HTSCs groups without using objective function logarithmic changes. Results also prove the differences among these classes for Molecular Effect Model (MEM) previously developed 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 (TC). Tikhonov Regularization (TR), Inverse Least Squares (ILS), Electronics Superconductors, High-Temperature Superconductors (HTSC), BCS Theory, Cuprates HTSCs [Hg-Ba-Ca-Cu-O] , [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.

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INTRODUCTION

The objective of this continuing study is to apply Artificial Intelligence by using Evolutionary Algorithms for modelling of several HTSCs classes. Namely, Hg-Cuprates, [Hg-Ba-Ca-Cu-O] constrained to $T_c > 0^\circ$], and improve/review Tin (Sn) group with $T_c > 0^\circ$], and Thallium (Tl) class subject to $[T_C < 0^\circ, T_C > 0^\circ]$ in Molecular Effect Model (MEM). The methods applied are 2D/3D Graphical Optimization and Genetic Algorithm techniques. All the software developed constitutes improvements/applications of previous research publications [3-9,48,49,50], not limited to Superconductors field. Along the GA optimization series published, Evolutionary Algorithms have proven be accurate and practical, with many programming options. Given any HTSCs class, if differences of molecular weight as a result of proportion/isotopic-variation in the molecule occur, the MEM, as an hypothesis to approximate/predict the T_c magnitude changes may be useful/efficacious. MEM was initially created on the basis of largely proven Isotope Effect. Inverse Methods, [3-9,48,49,50], could also be applied to select a desired T_c with optimal molecular weight composition in MEM. The innovations of this following research are given by the software for AI-GA methods. As was presented in [51], the advance consists in setting at Z axis the absolute difference between MEM T_C and experimental T_C . The software method applied in this study is set with GA Matlab tools and Imaging Processing programming. Results cogency involve GA MEM for Hg-Cuprates , and review with further explanations for Tin and Thallium HTSCs classes. 2D/3D GA Graphics of program performance, and final T_c polynomial predictive equations [3-5,48-51]. Succintly, the article shows an evolutionary algorithm method with 2D/3D Graphical Optimization for several HTSCs classes. The aim is to continue the improvements for MEM in search for refinements and precision. Applications in Electronics Physics new materials are explored.

MATHEMATICAL AND COMPUTATIONAL METHOD

At Tables 1-4, the software programming setting data for Equation (1) the programming algorithm made [3-5,48-51]. The Tikhonov Functional is implemented/improved with Chebyshev L_1 norm from previous research [48-51], Equation 1. As in [51], the difference with previous publications is the setting of MEM algorithm objective function at Z axis \lceil abs (T_C Experimental- T_C MEM \vert) in Figures 2-17. The dataset was applied in single and/or multifunctional charts into GA program. For Hg-Cuprates, first stage method, Figure 1, comprises the polynomial fit to obtain approximations for GA further programming constraints. Second stage is direct application of GA to get single/multifunctional graphics. Third stage is more difficult, consists in implementation of GA results into 3D Graphical optimization charts. With GA program, the refinements to obtain the MEM optimal fitness sectors are got.

EVOLUTIONARY ALGORITHMS MOLECULAR EFFECT MODEL OPTIMIZATION FOR HIGH TEMPERATURE SUPERCONDUCTORS CUPRATES AND REVIEW OF TIN AND THALLIUM CLASSES **Table: 2 - The literature optimization of classic parameters for [Sn-Sb-Te-Ba-Mn-Cu-O] class implemented [1,3-5,12-15,48-51]. This table is taken from [1,3-5,12-15,48-51] as the numerical initial data is the same for different mathematical-computational task.**

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Table 3.- The optimization of classic parameters for Thallium Molecular HTSC Group, [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] implemented, [1,3-5,12-15,48-50], subject to [$T_c > 0^\circ$ **C].**

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EVOLUTIONARY ALGORITHMS MOLECULAR EFFECT MODEL OPTIMIZATION FOR HIGH TEMPERATURE SUPERCONDUCTORS CUPRATES AND REVIEW OF TIN AND THALLIUM CLASSES **Table 4.- The classical optimization parameters for Thallium Molecular HTSC Class, [Tl-Sn-Pb-Ba-Si-Mn-Mg-Cu-O] implemented in this research [1,3-5,12-15,48-51] subject to [T^C** $< 0^\circ C$].

Algorithms and GA-Programming Method

Tikhonov algorithms have been extensively set in previous contributions [3-6, 48-51], both with L_1 Chevyshev norm and L_2 one. For this Molecular Model, the constraints values for parameters are shown in Tables 1-4. Sketch 1 shows the programming method for the following formula. The algorithms set for GA Molecular Effect, combined with a polynomial $p(MO_i)$ fits read,

minimize Tikhonov functional $J(\alpha)$ with α 1 = 0 and L₂ Norm, $J_{\alpha}(u)_{u \in \mathbb{R}} = |Au - MO|_1 + [\alpha 1] J(u)$; Hence minimize Chebyshev Norm, $\left|T_{\text{Ci}}-p(\text{MO}_{i})\right|_{1}$, for $i = 1,...,n$ subject to, $a \leq MO_i \leq a_1$; $b \leq T_{Ci} \leq b_1$;

 (1)

where

 $J_{\alpha}(u)$: Functional with regularization parameter alpha.

R : Real space.

u : Searched parameter solution.

MO_i: Molecular mass for Hg-Cuprates, Sn and TI HTSCs classes. Tables 1-4.

P(MO_i): Polynomial optimization parameter matrix. HTSC Hg-Cuprates, Sn and TI ranges, Tables 1-4.

a1 : Constant parameter. Tikhonov Regularization Parameter, selected null.

| • |: L₁ Chevyshev Norm (at algorithm software pattern set on absolute value).

a,a₁ : Constraints range specified at Tables 1-4 for HTSCs Hg-Cuprates, Sn and TI classes.

b, b₁: Constraints range specified at Tables 1-4 for HTSCs Hg-Cuprates, Sn and TI classes.

The programming techniques are related to previous research [3-9,48-51] and dual-program design [50,51]. In [49-51], software and imaging processing details with explanations are included. With the 2D polynomial fit data, it is possible to get approximations for further setting of GA constraints and lower/upper boundaries. Sketch 1 shows the software method base.

Sketch 1.-Programming method that was applied in the study

RESULTS FOR Hg-CUPRATES CLASS

Results for Hg-Cuprates are presented in Figs 1-9. By observing and guessing data from the figures series, it is easy going to learn and deduce all the graphical and numerical results. Hg-Cuprates MEM show get the most accurate results at present hypothesis stage.

Figure 1.-Among all the HTSCs studied in publication series, Hg-Cuprates MEM shows the best analytic geometry results. Note the close coincidence among splines and polynomial model. The GA programming multifunctional 2D graph. 2D Sn polynomial fit parameters intervals set into GA program with Matlab. As it was found in previous contributions, for Sn class the MEM shows in [48-51] an approximate 2D parabolic shape [3-5,48-51]. But Thallium class has a 2D sigmoid analytic geometry.

Figure 2.-Best Fit, with 5 optimization parameters, the most important chart of GA method. Generations Number is 300. As it was found in previous contributions, for Sn and Thallium classes the MEM shows in [50,51] an approximate 2D parabolic shape in 3D charts, Figs 8-9, [3- 5,48-51].

Figure 3.-The second most important 2D GA programming graph, note (% criteria met). Generations Number is 300. As it was found in previous contributions, for Sn and Thallium classes, the MEM shows in [50-51] acceptable results [3-5,48-51].

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Figure 4. - A multifunctional 2D GA programming graph. Generations Number is 300. Complementary data for scores and best individuals

Figure 5.- A 2D GA programming graph. Generations Number is 300. Complementary data for children generations and best individuals

Figure 6.- A 2D GA programming complementary graph showing fitness of every individual. Generations Number is 300.

Figure 7.- A 2D GA programming complementary graph showing score histograms. Generations Number is 300.

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Figure 8.- Optimal MEM sector for Hg-Cuprates HTSCs class. Generations Number is 300. Green arrow zone, the almost exact fit, red arrow, inset, shows the approximately acceptable fit. Hg-Cuprates MEM shows be the best at this stage. Model fits approximately well between molecular weights interval $[500, 1400]$ for all values of T_C.

Figure 9.- Additional grayscale perspective for optimal MEM sector of Hg-Cuprates HTSCs class. Generations Number is 300. Hg-Cuprates MEM shows be the best at this stage. Model fits approximately well between molecular weights interval $[500, 1400]$ for all values of T_C.

REVIEW WITH EXTENSIVE RESULTS FOR TIN AND THALLIUM MEM

This section is a review with further explanations from [51] database for Tin (Sn) and Thallium HTSCs classes. First part is Tin 2D/3D Graphical Optimization results, Figures 10-12 (erratum, at images is written Thallium in Figs 11-12, but the image correspond to Sn class). Second part corresponds to Thallium 2D/3D imaging charts, Figures 13-16. Multifunctional GA charts are shown for every HTSCs class. Brief of numerical results for both HTSCs classes is included in Table 6.

2D/3D Review of Results Sn GA Optimization

Figure 11 shows the 2D GA polynomial model in a multifunctional chart like in [48-51]. Figure 12 presents the optimal model sector for this MEM. The optimal zones for model are marked inset with arrows. Figure 12 represents MEM Tin HTSCs model in simple grayscale. The accuracy of these results are acceptable approximately, but Hg-Cuprates MEM fits better. 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 10 and 13 verify the GA program performance in a multifunctional chart. The most important graphs are the Best Fit that gives the fitness optimality, 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, as in Figures 2-7. This type of software was initially developed in [48-51].

Figure 10.-The Sn GA programming multifunctional 2D graph. 2D Sn polynomial fit parameters intervals set into GA program. Generations Number is 800. As it was found in previous contributions, for Sn class the MEM shows in [50,51] an approximate 2D parabolic shape [3- 5,48,49,50,51].

Figure 11.-Optimal MEM sector for Tin HTSC class. It was set as in [50,51] a 2-Degree polynomial MEM model, Table 6 . 2D polynomial fit parameters intervals were obtained from GA program. 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 [3-5,48,49,50,51]. Model fits approximately well between molecular weights interval [3200 , 4700] for all values of T_C. (erratum, at images is written Thallium in Figs 11-12, but the image correspond to Sn class) .

Figure 12.- 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. 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 [3-5,48,49,50,51]. Model fits approximately well between molecular weights interval $\lceil 3200, 4700 \rceil$ for all values of T_c . (erratum, at images is written Thallium in Figs 11-12, but the image correspond to Sn class) .

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

Figures 13-16 show Thallium AI programming results. Best sectors for MEM in Thallium class

are marked inset along the images.

Figure 13.- Similar method than Figs 2-7, but in multifunctional graph. The Thallium HTSCs class GA programming multifunctional 2D graph shows the most important GA optimization dataset. 2D Tl polynomial fit parameters intervals set into GA program. Generations Number is 800. Best fit with 3-Degrees polynomial line, Table 6, inset first graph. As it was found in previous contributions, for Tl class the MEM shows in [50,51] an approximate 2D sigmoidal analytic geometry shape [3-5,48-51].

Figure 14.- Optimal MEM sector for Thallium HTSC class. It was set as in [48-51] a 3-Degree polynomial MEM model. 2D polynomial fit parameters intervals were obtained from GA program. Generations Number is 500-800 for getting these polynomial coefficients. For Tl class the MEM shows get an approximate 2D sigmoidal shape [3-5,48-51]. Model fits approximately well between MEM temperatures interval [0,75] Centigrades for all values of Molecular Mass.

Figure 15.- From [51], a reviewed image processing with different perspective and optimal sector marked inset. Optimal MEM sector for Thallium HTSC class is approximately wide. It was set as in [48-51] a 3-Degree polynomial MEM model. 2D polynomial fit parameters intervals were obtained from GA program in Figure 4. Generations Number is 500-800 for getting these polynomial coefficients. Model fits approximately well between MEM temperatures interval [0 , 75] Centigrades for all values of Molecular Mass.

Figure 16.- From [51], a reviewed image with other image processing perspective and 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. 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] Centigrades for all values of Molecular Mass.

Numerical Results for Hg-Cuprates and Review of Sn and Tl Classes

Tables 5-6 show all the dual numerical results with errors for every HTSCs classes. Hg-Cuprates formula is almost quadratic. Errors can be considered acceptable. Number of GA generations is 300-800. Usually, polynomial coefficients of magnitude order about 10^{-9} are discarded for setting images.

Table 5.- From [51], 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.

Table 6. - From [51], brief of Numerical results for both HTSCs classes MEM optimization (polynomial) in 2D/3D Graphical GA implementation of software. In contrast with Hg-Cuprates, the formula obtained was approximated to quadratic. 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 residuals can be considered acceptable.

ELECTRONICS PHYSICS APPLICATIONS

From [51], Table 7 shows overview of applications for MEM one. Molecular Effect applications are guessed and developed from experimental literature database [3-5,38-51]. From Table 7, the following points can be considered important:

- 1. Every HTSCs class shows get a proper 2D algorithm according to Molecular Mass.
- 2. The most frequent analytic geometry shape obtained is inverse-parabolic.
- 3. Inverse methods can be applied for engineering design of Superconducting Multifunctional Transmission Lines [Casanovas, 2021].
- 4. Applications are at this stage theoretically deduced [3-5, 14, 15, 28, 48-51] . MEM usages were also detailed in previous contributions [48-51].

Table 7.-From [48-51], brief of applications for the MEM that were explained in former contribution series [3-5,48-51].

DISCUSSION AND CONCLUSIONS

This research objective was multiple. Firstly, to apply the Artificial Intelligence GA MEM on Hg-Cuprates HTSCs class, following the former study [51]. Secondly, review, improve, and compare this Hg-Cuprates class to Tin HTSCs class, subject to $T_c > 0^\circ$], and Thallium one, for $T_c <$ 0° , $T_c > 0^{\circ}$]. As in [51], the innovation of this study is the GA application following results got in previous contributions [3-5,48-51] . The GA optimization for Hg-Cuprates was performed with 5 parameters.

Results comprise Hg-Cuprates HTSCs class 2D/3D MEM polynomial Objective Function Graphical and Numerical Optimization database. These 3D imaging processing prove close similarities in MEM with the Tin class approximately parabolic-shaped curvatures and numericalgraphical extrapolations for T_c . The best results for MEM are got with the Hg-Cuprates group.

Numerical results for both HTSCs groups are approximately acceptable, Tables 5-6. These HTSC groups MEM [Casesnoves, 2020], 2D analytical geometry shapes and 3D MEM Objective Functions curvatures can be considered approximately satisfactory with low residuals, Figures 1- 16. Electronics Physics applications for MEM are explained, Table 7.

Advantages of this GA software method are the 2D/3D improved mathematical and geometrical numerical analysis for the MEM optimization. Further, the numerical coincidence with 2D polynomial fits proves the cogency of the Artificial intelligence method. 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, 39,48-51]. MEM hypothesis algorithms are at primary development stage.

Software and programming methods arebased on previous contributions [3-9, 48-51]. Sketch 1 shows the basic technique stages. The programming for Figures 1-9 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 Hg-Cuprates and Tin and Thallium HTSCs classes have been developed for MEM. Primary applications in Electronics/ Electromagnetic are included.

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Method is accepted by scientific community as an innovative dynamics method in deformable solids with mechanical, biomechanical and aerospace applications. New applications of this method will be probably found significantly in future.

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