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Genetic Algorithms Optimization for High Temperature Superconductors SN Class Molecular Effect Model with Electronics Applications

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Abstract

This contribution deals with the Molecular Effect Model (MEM) Genetic Algorithms polynomial-dual optimization for High Temperature Superconductors (HTSCs) class of [Sn-Sb-Te-Ba-Mn-Cu-O] . Results comprise Tikhonov Regularization Functionals development and mathematical methods for this HTSCs group without using logarithmic changes. Findings for this MEM optimization, based on Genetic Algorithms polynomial-dual-method show acceptable theoretical Numerical and 2D/3D Graphical Optimization solutions and low residuals. Solutions comprise two parts, the modelling for T_C Molecular Effect predictions equations, and 2D graphics series of results. Electronics Physics applications for Superconductors and High Temperature Superconductors are specified for Isotope Effect in BCS theory and for MEM and presented.

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

INTRODUCTION

In superconductors research series, ILS method was widely applied [3-6,39-49]. Genetic Algorithms (GA) method was applied on Hg-Cuprates HTSC class [3-5,48,49] with acceptable results. GA have proven be useful and efficacious in optimization and large-scale optimization [3-9]. Comparative optimization algorithms and methods constitute a practical tool for getting theoretical/experimental results confirmed [3-6, 39-49].

In previous studies, primary optimization for recent HTSCs with $T_C > 0°$ centigrade was presented. The definition of Temperature Superconductors [3-5] is those specific Superconductors whose Tc is approximately higher than 80 K—exactly 77 K [3-5, 12-15]. Their chemical molecular composition is complex with rather high molecular mass/weight and a number of groups/varieties. The fast improvements in HTSCs class research make a steady increasing number of new compounds, physical-chemical properties, and innovative applications. These HTSCs belong to Type II ones. In this contribution, the Molecular Effect Model predictive equation for HTSCs [Sn-Sb-Te-Ba-Mn-Cu-O] group are analyzed and examined.

The classical simple Isotope Effect Model, BCS theory, is a simple algorithm based on element-atomic mass of a Type 1 superconductor-element isotope and the Critical Temperature Tc [39-49]. That is, two main parameters and a constant to be determined experimental-numerically. That model has proven be acceptable with some inaccuracies [3-6, 39-49]. Previously, Isotope Effect and Molecular Effect hypothesis, [Casesnoves, 2020], was optimized with Genetic Algorithms dual-polynomial method for getting T_C predictions equation [standards, 48.49]. When deviations of molecular weight due to proportion/isotopic-variation in the molecule, the Molecular Effect mathematical model to predict the T_C magnitude changes for every HTSC group compound may be useful/efficacious, Tables 3-4. ***Grosso modo***, both Isotope Effect and MEM result be useful for T_C prediction equations in Superconductors and HTSCs. However, the second one is still hypothetical [48,49].

The software method applied in this study is dual. The first program is 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

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GA second program. The main advantage of this method is make sure of the numerical results cogency.

Results comprise MEM for this Sn class 2D charts, 2D GA Graphics of program performance, and final T_C polynomial predictive equations. The novelty of this study, is therefore, the GA application in contrast with previous contributions [3-5,48,49]

In summary, the article shows a 2D numerical-dual-graphical Genetic Algorithm Optimization study for the primary hypothesis of MEM set on [Sn-Sb-Te-Ba-Mn-Cu-O] HTSCs class. Algorithms are implemented with Matlab software and 2D Graphical model plots are also developed with this system. Both 2D numerical polynomial results and Genetic Algorithms software show low errors and residuals. The model analytic geometry shape results be an approximately parabolic curves.

MATHEMATICAL AND COMPUTATIONAL METHOD

Table 1 shows the software implementation data and Equation (1) the programming algorithm implemented. The Tikhonov Functional is developed/based from previous studies [49], Equation 1. The difference with other previous studies is the setting of algorithm into GA program. First stage method comprises the polynomial fit to obtain approximate parameter intervals to be implemented into the second stage GA program. With GA program, the refinement to obtain the final equation is done. The program method Flow Chart is shown in Sketch 1.

NUMERICAL OPTIMIZATION DATA FOR Sn-Sb-Te-Ba-Mn-Cu-O GROUP [HT-SUPERCONDUCTOR, MOLECULAR EFFECT HYPOTHESIS]	
FORMULATION	**MOLECULAR WEIGHT (UAM) / APPROXIMATE Tc (Kelvin)**
$Sn_{10}SbTe_9Ba_2MnCu_{21}O_{42+}$	4.7940e+003 / +187 C
$Sn_9SbTe_8Ba_2MnCu_{19}O_{38+}$	4.3565e+003 / +187 C
$Sn_8SbTe_7Ba_2MnCu_{17}O_{34+}$	3.9190e+003 / +167 C
$Sn_7SbTe_6Ba_2MnCu_{15}O_{30+}$	3.4816e+003 / +155 C
$Sn_{10}SbTe_4Ba_2MnCu_{16}O_{32+}$	3.6778e+003 / +141 C
$Sn_9SbTe_4Ba_2MnCu_{15}O_{30+}$	3.4635e+003 / +136 C
$Sn_8SbTe_4Ba_2MnCu_{14}O_{28+}$	3.2493e+003 /+129 C
$Sn_9SbTe_3Ba_2MnCu_{14}O_{28+}$	3.2403e+003 / +121 C

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]. This table is taken from [1] as the numerical initial data is the same for different mathematical-computational task.

For this Molecular Model, the constraints values for parameters are shown in Tables 1-4. The algorithms set for ILS Molecular Effect, with a polynomial $p(MO_i)$ read,

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

where

J_α (u) : Functional with regularization parameter alpha.
R : Real space.
u : Searched parameter solution.
MO_i : Molecular mass for HTSC Sn class.Table 1.
$P(MO_i)$: Polynomial optimization parameter matrix. HTSC Sn range Table 1.
α1 : Constant parameter. Tikhonov Regularization Parameter, selected null.
| • |: L_1 Chevyshev Norm (at algorithm software absolute value).
a,a_1 : Constraint range specified at Table 1 for HTSC Sn class.
b, b_1 : Constraint range specified at Table 1 for HTSC Sn class.

Programming Dual-method Flow Chart

Sketch 1shows the basic dual-program design. In [49], initial software was developed to form the base of this new one.

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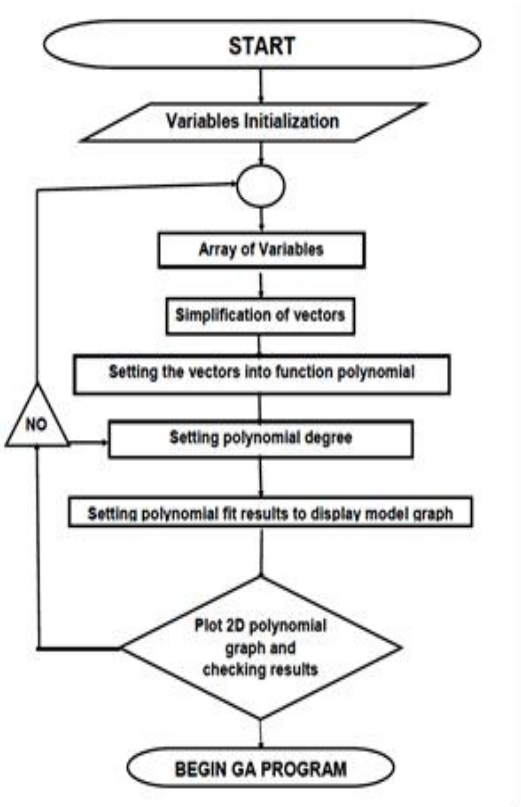
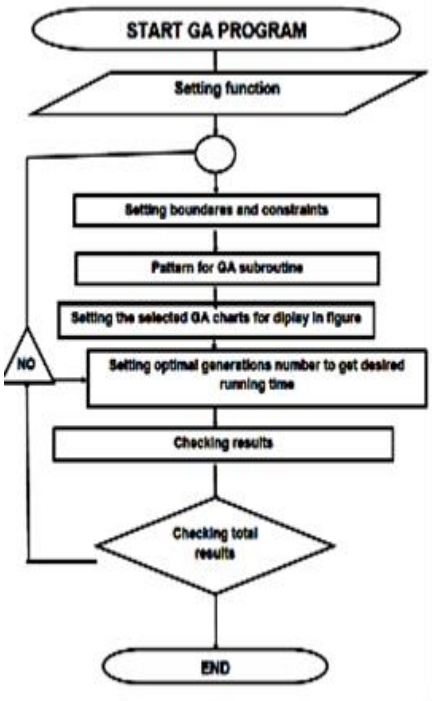
DUAL SOFTWARE FLOW CHART





Sketch 1.-Basic program structure simplified.

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RESULTS

The results are set into two stages. Figure 1 shows the First one 2D polynomial part. Figure 2 presents the GA results with the designed software. Numerical results are explained in Table 2.

Results Stage 1, Polynomial Optimization

Figure 1 shows in green the 2D polynomial model. Inset, red splines join the experimental data connected with model curve. This parabolic analytic geometry was obtained in previous research with ILS method [48,49].

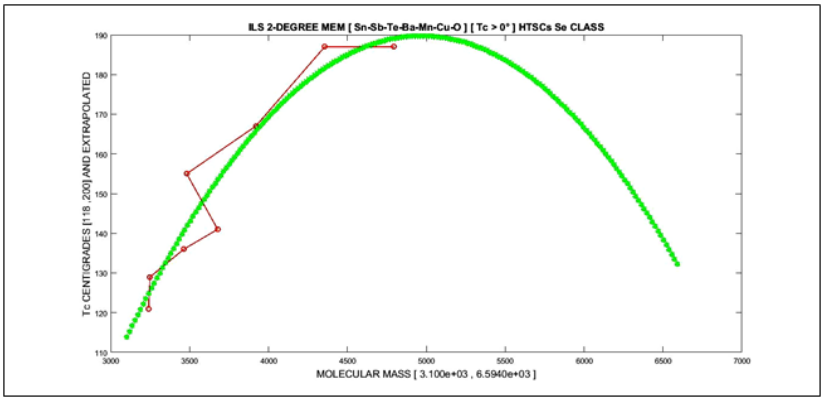

Figure 1.-2D polynomial fit with Matlab. As it was found in previous contributions, for Sn class the MEM shows get an approximate parabolic shape. Green extrapolated model, red, experimental dataset.

Results Stage 2, Genetic Algorithm

Figure 2 proves 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 [49].

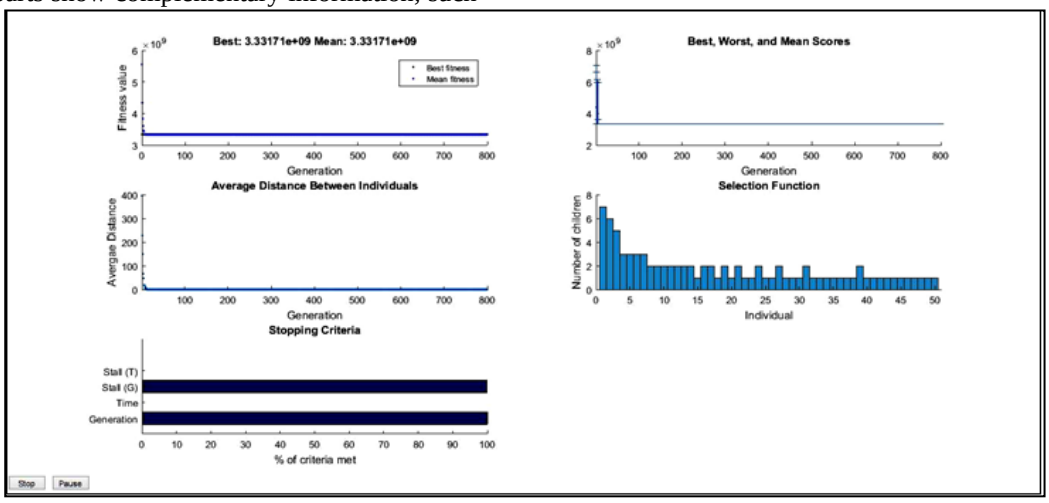

Figure 2.-The Second stage. 2D polynomial fit parameters intervals set into GA program with Matlab. Generations Number is 800. As it was found in previous contributions, for Sn class the MEM shows get an approximate 2D parabolic shape.

Numerical Results

Table 2 shows all the dual numerical results with errors. Errors can be considered acceptable. Note the 800 number of GA generations.

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NUMERICAL RESULTS		
STAGE	**METHOD**	**COMMENTS**
FIRST	Polynomial fit Inverse Least Squares	Program and 2D graphics patterns [Figure 1]
SECOND	Genetic Algorithm Tikhonov Functional	Program and Multigraphics pattern [Figure 2]
POLYNOMIAL MEM EQUATION		
Tc = [-21.7822e-006] + [216.4114e-003] MO + … **… +[-347.6922] MO^2**		**ERROR [200 functions]** **4.52E+00**
GENETIC ALGORITHM MEM EQUATION		
Tc = [-20.7821e-006] + [217.4114e-003] MO + … **… +[-346.6922] MO^2**		**ERROR [800 generations]** **5.77E+04**

Table 2.- Brief of Numerical results for optimization stage 1 (polynomial) and stage 2 (GA implementation) of software. Error is higher in GA because for GA the program was done for 800 generations, and for polynomial fit was made for 200 functions.

APPLICATIONS

Tables 3-4 overview of applications for Isotope Effect model and MEM one. Isotope Effect applications are confirmed in experimental literature database [3-5,39-49]. Isotope Effect applications have been experimentally and theoretically developed along decades [3-5,14,15,28,39-49] . MEM applications are hypothetical [48,49].

ISOTOPE EFFECT BCS MODEL APPLICATIONS		
APPLICATION TYPE	**METHOD**	**COMMENTS**
Usage of dataset for more different T_C formulas/algorithms [3-8]	Those other models are less simple	Dataset for one model could be useful for other model in first instance
Mixed element with different isotopes proportions	Optimization for the best T_C magnitude	This can be done with several optimization methods/algorithms [3-9, 39-49]
Element with unique isotope compound	Optimization for the best T_C magnitude for that exclusive isotope	This can be done with several optimization methods/algorithms [3-5, 39-49]
Simulations for both above types	Predictions for approximated T_C magnitudes	Several algorithms

Table 3.-Applications of the BCS isotope model that was developed in contribution series [3-5,48,49].

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SUPERCONDUCTING MOLECULAR EFFECT APPLICATIONS [HYPOTHESIS]		
TYPE	**USAGE**	**COMMENTS**
General 2D T_C / Molecular Mass curve shape	For catching up the approximate variation of T_C related to Molecular Mass. This is useful for guess of possibility of T_C predictions	Every HTSC class shows get a proper 2D shape. Usually parabolic inverse, but sigmoid can occur also [Thallium class, 3-8,39-49]
When there are several isotopes types in different proportions in the sample that cause variations in Molecular Mass	In this case, approximations/predictions for T_C could be got from the 2D curve equation	Approximations to be confirmed by following experimental data
When there are several isotopes types in different valences in the sample that cause a different Molecule within the HTSC class	In this case, approximations/predictions for T_C could be got from the 2D curve equation	Approximations to be confirmed by following experimental data. More difficult
When both phenomena happen. Different valences, and isotopes proportions in the prospective HTSC experimental work.	In this case, approximations/predictions for T_C could be got from the 2D curve equation	Much more difficult
Inverse Optimization of isotopes proportion to obtain a desirable T_C	Precision to reach an optimal T_C	This is a theoretical approach

Table 4.-Applications of the MEM that was developed in contribution series [3-5,48,49].

DISCUSSION AND CONCLUSIONS

This research objective was to prove/show the Genetic Algorithm Dual-Polynomial Optimization method for prediction results for MEM in HTSCs group [Sn-Sb-Te-Ba-Mn-Cu-O], subject to [$T_C > 0°$], Table 1. For this HTSCs group, MEM model was graphically, with polynomial-fitness, and numerically studied with GA Equation (1).

Results show two strands, 2D MEM polynomial fit with approximately parabolic-shaped curves and numerical-graphical extrapolations for T_C Numerical results for first optimization stage and second one match sharply and confirm one another their respective stages results. This HTSC group MEM [Casesnoves, 2020], can be considered acceptable with low residuals, Table 2, Figures 2-3. A number of applications for MEM and basic Isotope Effect BCS model are explained,Tables 3-4.

Advantages of this dual-method are the improved mathematical and geometrical numerical analysis for the optimization. An inconvenient with GA programming was the increasing running time when several GA optimization parameters are set in an unique graph.

Software methods and programming was based on previous contributions [3-9]. Specific subroutines and patters for every graph and numerical predictions table were built. The programming for Fig 2 requires arranging of GA special patterns loops, and setting precise upper and lower boundary limits for constraints.

Succintly, a 2D dual-polynomial GA methods for HTSCs group [Sn-Sb-Te-Ba-Mn-Cu-O] have been presented for MEM. Applications in Electronics Physics emerge from the study findings.

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. The GA nonlinear optimization software was invented/improved from previous contributions in subroutines modifications, patters, loops, graphics and optimal visualization [49]. At Method section, algorithm for basic Tikhonov Functional was developed from [3-5,48,49]. 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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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). 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 65 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 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).