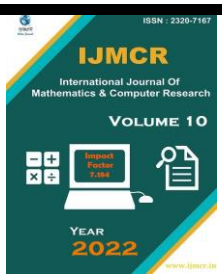
International Journal of Mathematics and Computer Research

ISSN: 2320-7167

Volume 10 Issue 04 April 2022, Page no. – 2662-2667

Index Copernicus ICV: 57.55, Impact Factor: 7.184

DOI: 10.47191/ijmcr/v10i4.05



Mathematical Optimization Molecular Effect Model Critical Temperature Predictions for High Temperature Superconductors with Electronics Physics Applications

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ARTICLE INFO

Published Online:
28 April 2022

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ABSTRACT

In previous series of contributions, Inverse Least Squares (ILS) 2D Numerical/Graphical Optimization for primary Molecular Effect model were presented. This contribution deals with the Molecular Effect Model predictions for High Temperature Superconductors (HTSCs) group of [Sn-Sb-Te-Ba-Mn-Cu-O] . This group constitutes a recent materials innovation of HTSCs with T_C > 0° with important recent/prospective electronics physics applications. For these optimization/simulations, classical Inverse Least Squares, 2D Interior Optimization, and 2D Graphical Optimization techniques are applied. Results comprise Tikhonov Regularization algorithms and mathematical methods for this HTSCs group. Findings for this Molecular Effect optimization, based on Inverse Least Squares and Inverse Least Squares polynomial methods show acceptable theoretical Numerical and 2D Graphical Optimization solutions and low residuals. Solutions comprise two parts, the modelling for T_C Molecular Effect predictions, and the Inverse Least Squares improved programming methods with 95% confidence intervals and statistical images. Proposed Electronics Physics applications for Superconductors and High Temperature Superconductors turn up from numerical/graphical results.

KEYWORDS: Interior Optimization (IO) Methods, 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).

I. MOLECULAR MODEL OPTIMIZATION INTRODUCTION

In a previous study, primary optimization for recent HTSCs with T_C > 0° centigrade was presented. Usually, [1-6, 14-16, 26-29], the classical High-Temperature Superconductors are those ones 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. These HTSCs belong to Type II ones.

In BCS classical superconductors theory, the Isotope Effect model [1-6, 14-16, 26-29] for uni-element superconductors equation reads,

$$[M_i]^{\alpha} T_C - K \cong 0; \quad \text{for } i = 1,....n; \tag{1}$$

where K is a constant, M Atomic Element Mass (AMU) of an element with (n) isotopes, T_C is critical temperature (Kelvin). (i) is the corresponding isotope for the element.

In this contribution, the Molecular Effect Model predictions for HTSCs [Sn-Sb-Te-Ba-Mn-Cu-O] group are presented. numerically-graphically shown [Casesnoves, 2020].

The Isotope Effect Model, Eq. (1), is a simple algorithm based on element-atomic mass of a Type 1 superconductor-element isotope and the Critical Temperature Tc. That is, two main parameters and a constant to be determined experimental-numerically. That model has proven be acceptable with some inaccuracies [3-5, 12-15]. In this study,

the Molecular Effect hypothesis, [Casesnoves, 2020], is optimizaed for getting T_C predictions.

The [Sn-Sb-Te-Ba-Mn-Cu-O] chemical group whose molecular composition/formulation diverge in proportion of valences/elements [1-9,12-15] is optimized with ILS polynomial model. From this theoretical-model base, predictive values of T_C are presented. When deviations of molecular weigth due to proportion/isotopic-variation in the molecule, the Molecular Effect mathematical model to predict the T_C magnitude change for every HTSC-group compound may be useful/efficacious.

In brief, the article shows a numerical-graphical optimization study for the primary hypothesis of Molecular Effect model set on [Sn-Sb-Te-Ba-Mn-Cu-O] HTSCs group. Algorithms are implemented with Matlab software and 2D Graphical model plots are also developed with this system. Both numerical results and 2D graphics show low errors and residuals. The model shapes results be an approximately parabolic curves.

II. MATHEMATICAL AND COMPUTATIONAL METHODS

What was needed is to set the Molecular Effect model for [Sn-Sb-Te-Ba-Mn-Cu-O] HTSC group was the molecular masses (MO) and the experimental T_C values, Table 1. The method is similar to [1], but in this study T_C predictions are obtained with software and graphical 2D statistical programming. Algorithm is based on Tikhonov Regularization Theory [12,13,31].

NUMERICAL OPTIMIZATION DATA FOR Sn-Sb-Te-Ba-Mn-Cu-O GROUP [HT-SUPERCONDUCTOR, MOLECULAR EFFECT HYPOTHESIS]

FORMULATION	MOLECULAR WEIGHT (UAM) / APPROXIMATE Tc Centigrade
$Sn_1OSbTe_9Ba_2MnCu_{21}O_{42+}$	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 [1,12-15]. This table is taken from [1] as the numerical initial data is the same for different mathematical-computational task.

For this Molecular Model predictions, the constraints values for parameters are shown in Tables 1-3. The algorithms set for ILS Molecular Effect, [1,13], with a polynomial p(MO) reads,

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

(2)

where MO is the molecular weight of the HTSC selected (i) within a HTSC group with (i) elements and [a-b] are constraints intervals. TC_i is critical temperature (Kelvin) for every (i) member of HTSCs group. The figure α1 is a constant specific Tikhonov Regularization Parameter, free to be appropiately selected. The constraints [a-b] are applied for optimization. OF was selected with ILS programming in Matlab without algorithmic-linearization with logarithms. Algorithm (2) programming with 2D imaging-processing results are shown in Figures 1-4.

The selected group of HRSCs constitutes a modern HTSC materials whose T_C is over 0° centigrades, with prospective applications [1-6, 14-16, 26-29]. Table 1 shows a narrow T_C differences interval, namely, approximately $T_{C\text{-}Group} \in$ [120,190] centigrades.

III. OPTIMIZATION RESULTS

Results are 2D Graphical and Numerical T_C predictions. Graphical results for 3-degree ILS polynomial model are shown in Figures 1,2. Matlab Graphical results for 4-degree ILS polynomial model are shown in Figures 3,4 with 95% statistical confidence interval. Both 3 and 4-degree show a parabolic shape for model. Numerical predictions are

presented in Tables [2,3], respectively for 3 and 4 ILS polynomial model. Errors can be considered acceptable and low.

ILS 3-Degree Model Results

Figs. 1,2 show parabolic-shaped curves for ILS 3-degree Molecular effect model in group of [Sn-Sb-Te-Ba-Mn-Cu-O] .

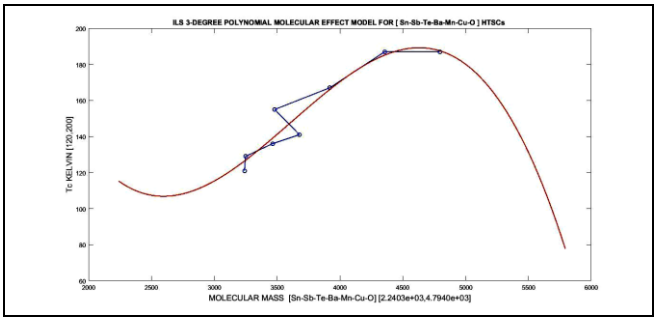

Fig. 1.- First 3-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Matlab Extrapolated modelled curve (red) and experimental data (blue). The model results to resemble a parabolic equation, approximately.

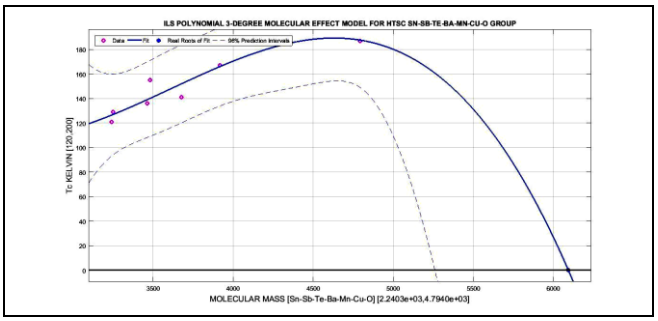

Fig. 2.- First 3-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (blue), confidence intervals (blue-dashed), and experimental data (red points). The model is a parabolic equation, approximately. Confidence Interval, blue-dashed-lines inset, is 95% , marked in dashed blue-lines parallel to model.

ILS 4-Degree Model Results

Figs. 3,4 show parabolic-shaped curves for ILS 4-degree Molecular effect model in group of [Sn-Sb-Te-Ba-Mn-Cu-O] .

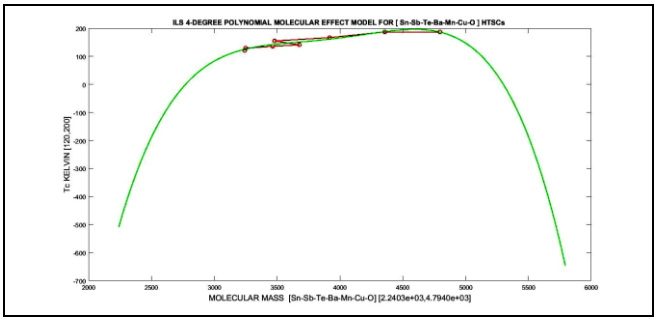

Fig. 3.- Second 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (green), and experimental data (red points). The model is a parabolic equation, approximately.

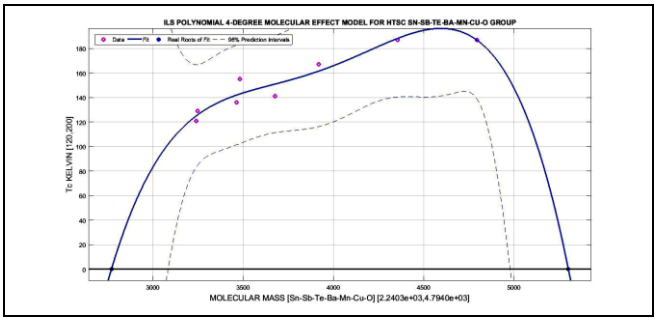

Fig. 4.- Second 4-degree ILS polynomial optimization of Molecular Effect Model for Sn-Sb-Te-Ba-Mn-Cu-O HTSCs group. Extrapolated modelled curve (blue), confidence intervals (blue-dashed), and experimental data (red points). The model is a parabolic equation, approximately. Confidence Interval, blue-dashed-lines inset, is 95% , marked in parallel to model.

ILS 3-Degree Model Predictions Results

Table 2 shows Numerical T_C predictions for ILS 3-degree model with errors. Predictions are numerically based on ILS polynomial 2D Graphical Optimization in Figs 1-4. Data obtained can be considered acceptable.

Table 2.- Numerical T_C predictions for ILS 3-degree model with errors ([T_C Experimental]-[T_C Predicted]) . The

OPTIMIZATION PREDICTIONS Tc MOLECULAR MODEL FOR [Sn-Sb-Te-Ba-Mn-Cu-O]	
MOLECULAR MASS	**Tc EXPERIMENTAL**
4794	187
4356.5	187
3919	167
3481.6	155
3677.8	141
3463.5	136
3249.3	129
3240.3	121
Tc PREDICTED	**ERROR [RESIDUAL 4.44320233780593]**
187.568123561098	-0.568123561098332
185.151755901108	1.848244098892
166.040208798827	0.959791201172607
140.069834151831	14.9301658481686
151.939414878914	-10.9394148789141
138.991341832237	-2.99134183223725
126.857143024242	2.14285697575804
126.382177851734	-5.38217785173424

software-development of parameters optimization for [Sn-Sb-Te-Ba-Mn-Cu-O] group requires appropriate patterns, loops and arrays. Data obtained can be considered acceptable. Note the numerical differences with ILS 4-degree model in Table 4, both in errors and residual.

ILS 4-Degree Model Predictions Results

Table 3 shows Numerical T_C predictions for ILS 3-degree model with errors. Predictions are numerically based on ILS polynomial 2D Graphical Optimization in Figs 1-4. Data obtained can be considered acceptable with lower errors/residual compared to ILS 3-degree model.

OPTIMIZATION PREDICTIONS Tc MOLECULAR MODEL FOR [Sn-Sb-Te-Ba-Mn-Cu-O]	
MOLECULAR MASS	Tc EXPERIMENTAL
4794	187
4356.5	187
3919	167
3481.6	155
3677.8	141
3463.5	136
3249.3	129
3240.3	121
Tc PREDICTED	ERROR [RESIDUAL 4.29102685700562]
186.827561856328	0.17243814367248
188.185961473922	-1.18596147392236
161.470460729484	5.52953927051567
142.816812530255	12.1831874697455
150.930540120149	-9.93054012014909
141.913885803682	-5.91388580368221
125.917530213279	3.08246978672105
124.937247272766	-3.9372472727664

Table 3.- Numerical T_C predictions for ILS 4-degree model with errors with errors ([T_C Experimental]-[T_C Predicted]) . The software-development of optimization of parameters for Sn-Sb-Te-Ba-Mn-Cu-O group requires appropriate patterns, loops and arrays. Data obtained can be considered acceptable. Numerical differences with ILS 3-degree model show lower error magnitudes and residual.

IV. DISCUSSION AND CONCLUSIONS

This research subject was to prove/show the prediction results for Molecular Effect Model in HTSCs group [Sn-Sb-Te-Ba-Mn-Cu-O]. This HTSCs materials are of interest because of their electronical-thermodynamical property with T_C > 0° . For this HTSCs group, Molecular Effect model was graphically and numerically studied.

Results have two strands, numerical-predictions for T_C and 2D graphical for model curves. Numerical-predictions are based on ILS 2D Graphical Optimization from Figs 1-4. Numerical results for this HTSC group Molecular Effect Algorithms [Casesnoves, 2020], can be considered acceptable with low residuals, Tables 2-3. Approximations with 3 and 4 degree ILS polynomial methods results have proven get low errors and residuals, Figs 1-4, Tables 2-3.

Software and programming was based on previous contributions [1-9, 17-25]. Specific subroutines and patters for every graph and numerical predictions table were built. The programming for Figs 2 and 4 requires statistical and confidence intervals patterns.

In summary, 2D ILS polynomial Graphical Optimization methods for HTSCs group [Sn-Sb-Te-Ba-Mn-Cu-O] predictions have primarily agreed to theoretical hypothesis. Applications in Electronics Physics emerge from the study findings.

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SCIENTIFIC ETHIC STANDARDS

Molecular Effect model was created by author in 2020-1. 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, from [1-10], whose inclusion is essential to make the contribution understandable. The 2D Graphical Optimization in Matlab constitutes a software engineering improvement from previous contributions [1,3-9]. 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 International Scientific Community and European Union Technology and Science Ethics [38-41]. References [40,41] and [38,39]: '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 [37-40]. 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, algorithm, 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].