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SUPPORT VECTOR REGRESSION APPROACH OF MODELING THE SUPERCONDUCTING TRANSITION TEMPERATURE OF BOROCARBIDE-BASED SUPERCONDUCTORS

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ABSTRACT

Perpetual current carrying ability of borocarbide-based superconductors renders it indispensable in many practical applications such as generation of high magnetic field. Coexistence of superconductivity and magnetism in this superconductor also allows deep understanding of the interaction between the two phenomena. The superconducting transition temperatures (T_C) of these compounds are very sensitive to Ni-Ni distance which is governed by the lattice parameter a that further controls the electronic structure of the Ni(3d) dominated conduction bands. For quick investigation of the effect of structural disorder (which could result from doping) on the T_C of these superconductors, we develop support vector regression (SVR)-based model that estimates the T_C of different borocarbide-based superconductors using lattice parameters descriptors. Comparison of the estimated T_C with the measured values shows excellent agreement. The outstanding performance demonstrated by the proposed SVR-based model in estimating the T_C of borocarbide-based superconductors indicates that the model can be adopted for quick estimation of T_C of fabricated borocarbides compounds thereby providing an excellent alternative to the use of sophisticated equipment which are costly and time consuming.

Keyword: borocarbide superconductor, support vector regression, superconducting transition temperature, lattice parameters.

1. INTRODUCTION

Discovery of superconductivity in intermetallic borocarbide (RNi_2B_2C; R= rare earth metals, Ni= transition metals) compounds attracted attention because of its relatively high transition temperature and its ability to coexist magnetism and superconductivity. Body-centered tetragonal $LuNi_2B_2C$ type was identified as superconducting phase of this compound in which R-C layers alternate with Ni_2B_2 layers and nickel remains tetrahedrally coordinated by four atoms of boron [1] [2]. Variation of Tc with the nearest neighbor in-plane Ni-Ni distance (governed by lattice parameter a) is established for RNi_2B_2C compounds [3]. Although, ionic radius of R seems to alter the T_C in these compounds, critical investigation shows that R atoms influence the T_C indirectly by their effect on in-plane and c-axis Ni-Ni distance which ultimately changes the electronic structure as well as the bandwidths of the Ni(3d) conduction bands [3]. Substitutions (such as Co substituted for Ni) suppress the T_C of RM_2B_2C materials with distortions in lattice parameters as evident in $HoCo_2B_2C$ and $HoNi_2B_2C$ compounds in which $HoCo_2B_2C$ shows no superconductivity down to 30mK [4]. These chemical substitutions distort lattice parameters which further bring about a reduction in density of states at Fermi level as well as weakening in electron- phonon coupling and thereby affect the T_C[4]. This work proposes SVR-based model as a novel computational intelligence model that directly estimates the T_C of various borocarbide superconductors with the aid of lattice parameters as descriptors.

Support vector regression (SVR) is an intelligence learning tool that implements kernel trick for non-linear problems [5]. SVR has proved its effectiveness in many practical applications since non-linearity characterizes many real life problems [6]. The algorithm has effectively handled material's surface properties[7]–[10], magnetic properties of manganite refrigerant [11]-[14] and superconducting properties of some materials [15]-[17] among others. Unique properties of SVR algorithm which include excellent generalization and predictive ability, optimal minimal convergence as well as its strong mathematical foundation lead to its choice in this present work. Implementation of the proposed model would be of immense significance in circumventing the experimental stress involved in determining T_C of borocarbide-based superconductors.

The correlation coefficient between the measured T_C of borocarbide-based superconductors and the estimated values obtained during the modeling and simulation show that the developed SVR-based model is capable of estimating T_C up to 95.44% accuracy. While deploying the developed model to other borocarbide-based superconductors that are not involved in training and testing phase of model development, the outcomes of the developed model agree excellently with the measured values.

2. BRIEF DESCRIPTION OF THE PROPOSED METHOD (SVR)

Support vector regression is a learning algorithm proposed by Vapnik to solve regression tasks [18]. SVR has a good sound mathematical framework that results in optimal solution for its optimization problem. In addition, SVR performs excellently by maintaining good generalization error when the input dataset is small as it does not over-fit. The input vector, $\boldsymbol{x}$, corresponds to the training dataset employed to train the SVR model and are first mapped to a high-dimensional feature space using a non-linear mapping function, $\varphi(\boldsymbol{x})$[19]. Linear regression is then performed on the transformed data in this high-dimensional space by constructing a set of hypothesis. The linear model of SVR can thus be expressed as:

$$g(\boldsymbol{x}, w) = \sum_{k=1}^{m} w_k \varphi(\boldsymbol{x})_k + b \quad (1)$$

where the w_k's are the model parameters and b is a bias term. The ε- insensitive loss function is proposed to evaluate the accuracy of the model and is defined as:

$$L_\varepsilon\big(y, g(\boldsymbol{x}, w)\big) = \begin{cases} 0, & if\ |y, g(\boldsymbol{x}, w)| \le \varepsilon \\ |y, g(\boldsymbol{x}, w)| - \varepsilon, & Otherwise \end{cases} \quad (2)$$

The ε parameter is used to specify the margin of error on the training data. An empirical risk function is defined by placing a theoretical bound on the model through averaging of the loss function over the whole training data. Thus, the empirical risk function is given in equation (3).

$$R_{emp}(w) = \frac{1}{m}\sum_{k=1}^{m} L_\varepsilon\big(y_k, g(\boldsymbol{x_k}, w)\big) \quad (3)$$

An hypothesis which minimizes the above risk function is chosen to formulate the optimization problem which is then solved by the SVR model.

The generalization error of SVR depends on the optimum combination of its user-defined three parameters namely regularization parameter C, epsilon ε and kernel specific function. Regularization parameter maintains a compromise between the model complexity and the error allowed on the training data with smaller errors corresponding to larger value of C and higher model complexity. The support vectors on the insensitive zones are controlled by the epsilon parameter while kernel function controls the transformation of the input data to the higher dimensional space where linear regression can be performed on the transformed data. These parameters are well optimized in this present work using test-set cross validation method.

3. EMPIRICAL STUDY

This section describes the data-set used for modeling and simulation. The computational description of the model is also presented.

3.1 Description of the dataset

A dataset containing thirty data-points was used for modeling SVR algorithm that estimates the T_C of several classes of borocarbide-based superconductors. The dataset consists of experimentally measured T_C of borocarbide superconductors and their corresponding lattice parameters as extracted from literature [20]-[28]. Statistical analysis was performed on the dataset and the outcomes of the analysis are shown in table 1. The mean of the dataset as well as the maximum and minimum are useful information through which the overall content of the dataset can be inferred. The standard deviations also show the level of discrepancies in the dataset. The standard deviations obtained from the dataset used for the present simulation show high level of consistence in the dataset. Similarly, the values of correlation coefficients presented in the table show that the lattice parameter descriptor along c-axis of the body-centered tetragonal is weakly correlated with superconducting transition temperature while lattice parameter descriptor along a-axis is linearly correlated with the target. Both coefficients of correlation show ineffectiveness of linear model in establishing a relationship between the descriptors.

Table-1. The results of the statistical analysis carried out on the dataset.

	a (pm)	**c** (pm)	**Tc** (K)
Mean	360.83	1057.78	10.8
Maximum	386.81	1086.00	16.8
Minimum	335.00	1022.00	2.5
Standard deviation	15.69	14.59	4.3
Correlation coefficient (%)	0.46	0.0907	

3.2 Computational methodology

The available dataset for the modeling was randomized and portioned into training and testing dataset prior to the commencement of the simulation task in MATLAB computing environment. Data randomization before separation into training and testing set ensures efficient computation and uniform distribution of dataset. SVR hyper-parameters which include the regularization factor, epsilon, kernel option and hyper-parameter lambda were optimized using test-set cross validation procedures described in [8]. The computational description of the developed SVR-based model can be summarized as follow:

Step 1: *Data randomization and separation*-The dataset for the modeling is randomized and separated into two sets (training and testing sets) in the ratio of four to one, respectively.

Step 2: *kernel function selection and hyper-parameters initialization*- A kernel function is selected (for example, Gaussian function, and polynomial, sigmoid among others) and the kernel parameter

(called kernel option) is initialized. Other hyper-parameters are also initialized.

Step 3: *Hyper-parameters optimization*- Random constant values are assigned to epsilon, hyper-parameter lambda and kernel option of a selected kernel function while the value of regularization factor is varied until high correlation coefficient is obtained between the measured superconducting transition temperature and the estimated results. Optimum value of regularization factor is established using the testing dataset on the SVR algorithm trained using training set of data. The optimum value of regularization factor is saved while the process is repeated for other hyper-parameters at the optimum value of each of the optimized parameters. The optimum values of each of the hyper-parameters are saved while the corresponding measures (root mean square error and mean absolute error) of model generalization and predictive strength are also saved.

Step 4: *Algorithm training using optimum hyper-parameters*-SVR algorithm is trained using the combination of the optimum values of all the hyper-parameters while the generalization and estimation capacity of the trained model is assessed using testing set of data. The optimum values of each of the hyper-parameters are presented in table 2 so as to enhance the reproducibility of the presented results.

Table-2. Optimum parameters for the proposed SVR model.

Hyper-parameter	Optimum value
Regularization factor (C)	42
Hyper-parameter(Lambda)	1E-7
Epsilon	0.009
Kernel option	2.18
Kernel function	Radial Basis Function

4. RESULTS AND DISCUSSIONS

This section discusses the results of the simulation and modeling. Measures of generalization and predictive strength of the developed SVR-based model are presented and discussed. The comparison of the results of the developed model is also compared with the measured values.

4.1. Generalization and predictive capacity of the developed SVR-based model

The predictive and generalization capacity of the developed SVR-based model for accurate and effective estimation of the superconducting transition temperature of borocarbide-based superconductors is assessed using correlation coefficient (CC), root mean square error (RMSE) and mean absolute error (MAE) for both training and testing dataset. Table 3 presents the values of the measures of model generalization and predictive capacity.

Table-3. Generalization performance evaluation parameters.

	Training	Testing
CC (%)	99.41	95.44
RMSE (K)	0.597	1.287
MAE (K)	0.227	0.905

4.2. Influence of lanthanides and actinidemetals on transition temperature of $XPt_2 B_2 C$ superconductor

The influence of some lanthanides metals as well as actinide metal on superconducting transition temperature of $XPt_2 B_2 C$ superconductor was investigated using the developed SVR-based model and the results of the model are depicted in Figure-1. $LaPt_2 B_2 C$ shows highest value of transition temperature in all the presented metals due to its lowest ionic radius as compared to others.

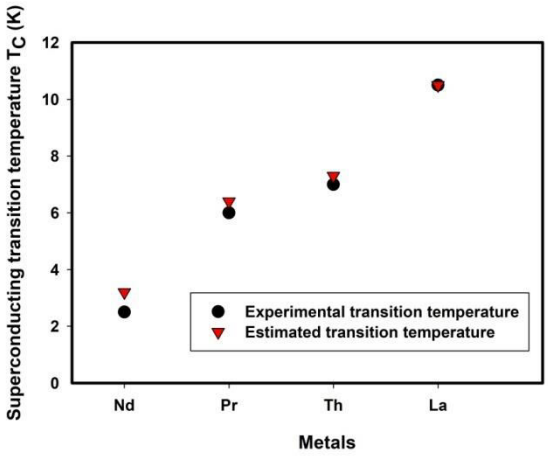

Fig.1: Effect of lanthanide and actinide metals on the superconducting property of $XPt_2 B_2C$ borocabide superconductor

It was observed that the transition temperature of $XPt_2 B_2 C$ decreases with increase in ionic radius of the metals. This similar trend has also been reported elsewhere [29].

4.3. Effect of transition metals, lanthanides and actinides on transition temperature of $XNi_2 B_2 C$ superconductor

Figure-2 presents the influence of transition metals (Scandium Sc and Yttrium Y), lanthanides (Dysprosium Dy, Erbium Er, Thulium Tm and Lutetium Lu) and thorium actinide metal on the superconducting transition temperature of $XNi_2 B_2 C$ superconductor. From the results of the developed SVR-based model, transition temperature increases with increase in the ionic radius of lanthanides. Similar trend is also observed for transition

metals. The results of the developed SVR-based model agree well with the reported experimental values[3], [30].

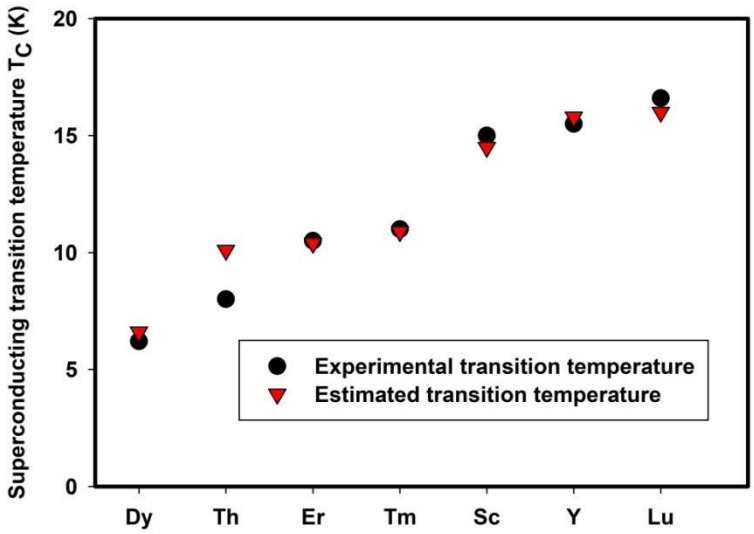

Fig.2: Effect of transition metal, lanthanide and actinide metals on the superconducting property of XNi_2B_2C borocabide superconductor

4.4. Influence of manganese on transition temperature of $Y(Ni_{1-X}Mn_X)_2 B_2 C$ superconductor

`The doping effect of manganese on the transition temperature of of $Y(Ni_{1-X}Mn_X)_2 B_2 C$ superconductor was also investigated using the developed model. The results of the model are compared with the experimentally measured values and show good agreement [2]. Figure-3 shows the comparison. It was found that manganese decreases the transition temperature of the superconductor. It should be noted that the developed model was only supplied with the descriptors in these implementations while the developed model utilizes its acquired support vectors during the training phase for its estimation.

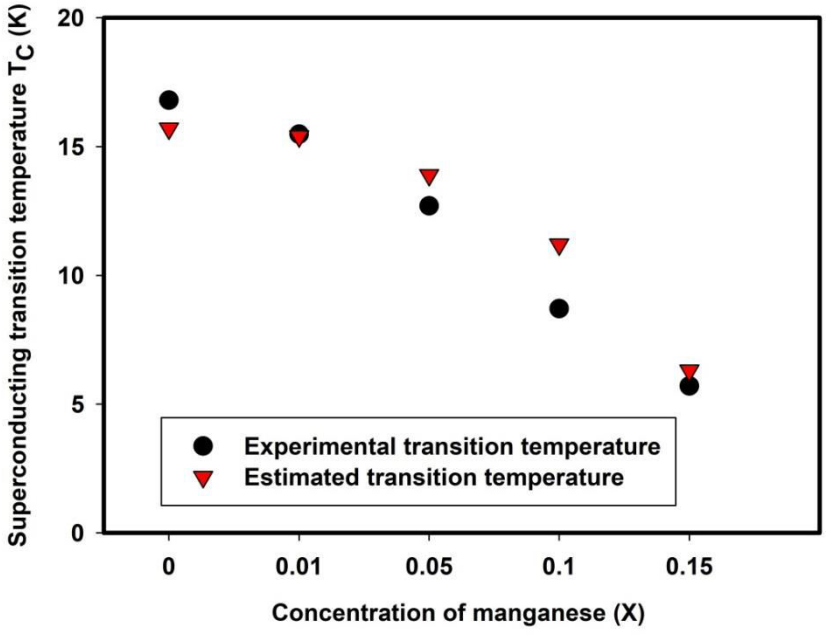

Fig. 3:Effect of maganese on the superconducting property of $Y(Ni_{1-X}Mn_X)_2B_2C$ borocarbide superconductor

5. CONCLUSION AND RECOMMENDATION

SVR was used to develop a model that estimates the T_C of different borocarbide-based superconductors via test-set cross validation technique. Comparison of the estimated T_C with experimental values shows excellent agreement. The outstanding performance of SVR shows that the model offers a viable means of strengthening the search of superconductivity in borocarbide compounds through quick estimation of the T_C of fabricated samples without the need for sophisticated equipment which may be costly and time consuming. As a result of the outstanding performance of SVR in predicting the T_C of these superconductors, we recommend the use of computational intelligence technique in estimating other superconducting properties of these compounds.

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