

Research Article

Computational Intelligence Approach for Estimating Superconducting Transition Temperature of Disordered MgB_2 Superconductors Using Room Temperature Resistivity

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Doping and fabrication conditions bring about disorder in MgB_2 superconductor and further influence its room temperature resistivity as well as its superconducting transition temperature (T_C). Existence of a model that directly estimates T_C of any doped MgB_2 superconductor from the room temperature resistivity would have immense significance since room temperature resistivity is easily measured using conventional resistivity measuring instrument and the experimental measurement of T_C wastes valuable resources and is confined to low temperature regime. This work develops a model, superconducting transition temperature estimator (STTE), that directly estimates T_C of disordered MgB_2 superconductors using room temperature resistivity as input to the model. STTE was developed through training and testing support vector regression (SVR) with ten experimental values of room temperature resistivity and their corresponding T_C using the best performance parameters obtained through test-set cross validation optimization technique. The developed STTE was used to estimate T_C of different disordered MgB_2 superconductors and the obtained results show excellent agreement with the reported experimental data. STTE can therefore be incorporated into resistivity measuring instruments for quick and direct estimation of T_C of disordered MgB_2 superconductors with high degree of accuracy.

1. Introduction

Superconductor is a material that allows perpetual flow of current as a result of disappearance of its electrical resistivity when it is cooled below a particular temperature called superconducting transition temperature (T_C). Several practical applications of superconductors such as magnetic resonance imaging in hospitals, magnetic levitation train, particle accelerators, superconducting quantum interference devices, magnetoencephalography, and filters for mobile communication and their future applications (which include transmission of electricity, fast computing, and high temperature superconducting generator) depend mainly on the value of T_C . Phenomenon of superconductivity was first observed in mercury in 1911 when electrical resistance of

pure mercury went to zero around 4 K [1]. Understanding of this behavior was not clearly known until 1957 when three physicists propounded BCS theory which governs the emergence of superconductivity [2]. This theory attributes the emergence of superconductivity in materials to the ability of electrons to pair (formation of cooper pairs) which pave ways for the free movement of electrons in a coordinated manner. Collision of electrons with lattice, other electrons, and defects among others bring about resistivity in materials and this is circumvented in superconductors due to the formation of cooper pairs. Efforts have been made to realize room temperature superconductor and to raise the values of T_C of known superconductors. However, MgB_2 holds a promising future since its T_C can be altered through doping and fabrication conditions [3–5].

The awareness of superconductivity in magnesium diboride (MgB_2) in 2001 marked a new advancement that diversifies the applications of superconductors [6]. MgB_2 is a two-band superconductor with several practical applications as a result of its unique properties such as transparency of the grain boundaries which permits flow of current, lower anisotropy, and large coherence length. Its economic affordability as well as its unique properties offers it a special place in practical applications despite its low T_C as compared with high temperature superconductors. The techniques that are usually employed for improving the superconducting properties of MgB_2 include introduction of disorder through chemical doping and several thermomechanical processing techniques which alter its room temperature resistivity [3, 5, 7–24]. In order to improve the superconducting properties of this material (in particular T_C), we develop STTE for accurate, quick, and direct estimation of T_C of disordered MgB_2 superconductors as an alternative to conventional method which is experimentally intensive. This developed model allows the potential of several dopants to be assessed within short period of time so as to ascertain the specific dopant that improves the superconducting property of MgB_2 superconductor.

The normal state strong electron-phonon scattering which gives rise to the large room temperature resistivity in intermetallic superconductors is associated with the observed high T_C [25]. Low resistivity of MgB_2 at room temperature and temperature just above its T_C could be attributed to its two-band nature characterized with different strength of electron-phonon coupling [25]. Its superconductivity comes from the large coupling in 2D σ band and MgB_2 demonstrates anisotropy in the normal state resistivity. The proposed SVR based model has been reported as a novel tool of estimating superconducting properties of doped MgB_2 superconductor using few descriptive features [26]. The choice of SVR in building STTE is due to its many unique features which include sound mathematical foundation, nonconvergence to local minima, accurate generalization, and predictive ability when trained with few descriptive features [27].

SVR tackles real life problems using the principles of artificial intelligence in the field of machine learning. It acquires pattern or relation that exists between the target (T_C) and descriptor (room temperature resistivity) and adopts the acquired pattern for future estimation of the unknown target with the aid of the descriptors. Its excellent predictive ability is made which is used in tackling several problems in medical field [28], material science [26, 29–32], and oil and gas industries [33, 34], to name but a few. The excellent predictive and generalization ability of SVR in solving numerous problems coupled with the need to have accurate, direct, and effective way of estimating the effects of disorder on T_C of MgB_2 superconductor serves as motivation for carrying out this research work.

2. Description of the Proposed Model

SVR follows a learning algorithm formulated from support vector machines which was originally proposed by Vapnik for classification purposes [35]. It uses loss function ε that

controls the smoothness of the response of SVR and the number of support vectors which ultimately affect the generalization capacity as well as the complexity of the model. The loss function ε represents the maximum error (deviation of the target vectors tolerated by the model). Equation (1) represents a linear decision function in which $\langle w, x \rangle$ indicates a dot product in space R^N :

$$f(x, \alpha) = \langle w, x \rangle + b, \quad (1)$$

where $w \in R^N$ (input space) and $b \in R$.

Minimization of Euclidean norm $\|w\|^2$ is necessary since flatness of the defined decision equation is desired. The optimization problem for the regression is presented in

$$\begin{aligned} & \frac{1}{2} \|w\|^2 \\ \text{Subject to } & y_i - \langle w, x_i \rangle - b \leq \varepsilon \\ & \langle w, x_i \rangle + b - y_i \leq \varepsilon. \end{aligned} \quad (2)$$

The assumption entailed in the optimization problem presented in (2) is the existence of a function that controls the error in all training pairs in such a way that the error is less than ε . In order to build up a robust system that caters for external constraints, slack variables (ξ and ξ') are introduced in the optimization problem and presented in [27]

$$\begin{aligned} & \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n (\xi_i + \xi'_i) \\ \text{Subject to } & y_i - \langle w \cdot y \rangle - b \leq \varepsilon + \xi \\ & \langle w \cdot y \rangle + b - y_i \leq \varepsilon + \xi' \\ & \xi', \xi \geq 0 \\ & \forall i = 1, 2, \dots, n. \end{aligned} \quad (3)$$

The regularization factor C introduced in (3) trades off the frequency of error and the complexity of decision rule by altering the size of slack variables.

The optimization problem is solved by using Lagrangian multipliers ($\lambda_i, \lambda'_i, \eta_i$, and η'_i) to transform the problem to dual space representation. The constraint equations are multiplied by the multipliers and the result is taken away from $\|w\|^2$ (objective function). The resulting Lagrangian is illustrated in

$$\begin{aligned} L = & \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n (\xi_i + \xi'_i) \\ & - \sum_{i=1}^n \lambda_i (\varepsilon + \xi_i - y_i + \langle w, x_i \rangle + b) \\ & - \sum_{i=1}^n \lambda'_i (\varepsilon + \xi'_i + y_i + \langle w, x_i \rangle - b) \end{aligned}$$

$$\begin{aligned}
& - \sum_{i=1}^n \lambda'_i (\varepsilon + \xi'_i + y_i - \langle w \cdot y \rangle - b) \\
& - \sum_{i=1}^n (\eta_i \xi_i + \eta'_i \xi'_i).
\end{aligned} \tag{4}$$

In order to obtain the solution of the optimization problem, the saddle points of the Lagrangian function are obtained by equating the partial derivative of Lagrangian with respect to w , b , ξ_i , and ξ'_i to zero which gives rise to (5) as described in [29]:

$$\begin{aligned}
w &= \sum_{i=1}^n (\lambda'_i - \lambda_i) \cdot x_i \\
\eta_i &= C - \lambda_i \\
\eta'_i &= C - \lambda'_i.
\end{aligned} \tag{5}$$

By putting (5) in (4), we have

$$\begin{aligned}
& - \frac{1}{2} \sum_{i,j=1}^n (\lambda'_i - \lambda_i) (\lambda'_j - \lambda_j) (x_i \cdot x_j) \\
& - \varepsilon \sum_{i=1}^n (\lambda'_i + \lambda_i) + \sum_{i=1}^n y_i (\lambda'_i - \lambda_i) = 0
\end{aligned} \tag{6}$$

$$\text{Subject to } \sum_{i,j=1}^n (\lambda'_i - \lambda_i) = 0 \quad \text{where } 0 \leq \lambda'_i, \lambda_i \leq C. \tag{7}$$

The estimation problem presented in (1) is finally represented by (8) after incorporating λ_i and λ'_i obtained from (6):

$$f(x, \alpha) = \sum_{i=1}^n (\lambda'_i - \lambda_i) K(x_i, x) + b. \tag{8}$$

Kernel function $K(x_i, x)$ represents a nonlinear mapping function that maps nonlinear regression problem to high dimensional feature space where linear regression is performed. The choice of kernel function depends on the nature of the problem and could be linear, polynomial, Gaussian, or sigmoid kernel function.

During the course of optimizing the SVR model, SVR variables such as the regularization factor (C), epsilon (ε), hyperparameter (λ), and kernel option were defined and adjusted until the model attained optimum performance.

The training stage of the proposed model entails acquisition of pattern that exists between the descriptor and the target which could further be generalized by the model so as to accurately estimate unknown target with the aid of the descriptor. High correlation coefficient, low root mean square error, and low mean absolute error signify the accuracy and efficiency of the model. In the case of STTE developed in this research work, the SVR model was taken through training and testing stages and then used to estimate T_C of several MgB₂ superconductors.

TABLE 1: The dataset used for modeling STTE.

Resistivity at room temperature ($\mu\Omega\text{-cm}$)	T_C (K)
29.800	38.50
27.500	39.20
35.00	38.80
17.000	38.90
9.600	39.40
17.992	38.50
48.000	38.80
29.250	35.70
45.684	34.50
7.800	41.00

2.1. Evaluation of the Performance of the Developed Model.

The performance of the developed model was evaluated on the basis of the correlation coefficient (CC) between the experimental and the estimated T_C , root mean square error (RMSE), and mean absolute error (MAE). The generalization performance was evaluated using

$$\begin{aligned}
\text{CC} &= \frac{\sum_{i=1}^n (Y_{i(\text{exp})} - Y'_{i(\text{exp})}) (Y_{i(\text{est})} - Y'_{i(\text{est})})}{\sqrt{\sum_{i=1}^n (Y_{i(\text{exp})} - Y'_{i(\text{exp})})^2 \sum_{i=1}^n (Y_{i(\text{est})} - Y'_{i(\text{est})})^2}} \\
\text{RMSE} &= \sqrt{\frac{1}{n} \sum_{i=1}^n e_i^2} \\
\text{MAE} &= \sum_{i=1}^n \frac{|e_i|}{n},
\end{aligned} \tag{9}$$

where e_i and n represent error (difference between the experimental and estimated T_C) and number of data points, respectively. $Y_{i(\text{exp})}$ and $Y_{i(\text{est})}$, respectively, represent the experimental and the estimated T_C , while $Y'_{i(\text{exp})}$ and $Y'_{i(\text{est})}$ represent their mean value, respectively.

In the case of the developed model, high correlation coefficient of 100%, low root mean square error of 1.29, and low absolute error of 0.279 were obtained during the testing phase of the model.

3. Empirical Study

3.1. Description of the Dataset. The dataset that was employed in modeling STTE comprises a total number of ten experimental values of room temperature resistivity and the corresponding T_C of disordered MgB₂ superconductors. The adopted dataset was drawn from the literatures [36–38] and presented in Table 1.

Statistical analysis was carried out on the dataset and the results of the analysis are presented in Table 2.

Deduction from the values of the mean, median, standard deviation, minimum, and maximum gives insight into the dataset as well as the level of its discrepancies. The correlation coefficient between T_C and room temperature resistivity was calculated and found negatively correlated. Meanwhile,

TABLE 2: Statistical analysis of the dataset used in modeling STTE.

	T_C (K)	Resistivity at room temperature ($\mu\Omega\text{-cm}$)
Mean	38.33	26.763
Median	38.33	28.375
Standard deviation	1.87	13.821
Maximum	41.00	48.000
Minimum	34.50	7.800
The coefficient of correlation between the target and descriptor is -0.6023		

the obtained correlation suggests the level of relationship between the target and descriptor.

3.2. Computational Methodology. The modeling and simulations involved in this work were conducted within the computing environment of MATLAB. The dataset presented in Table 1 was randomized prior to the commencement of the modeling. The randomization was carried out purposely to enhance computational efficiency and to ensure consistency. The dataset was further divided into training and testing set in the ratio of 8 to 2. The best values of SVR hyperparameters (i.e., regularization factor, kernel option, lambda, and epsilon) were used for generating support vectors through training dataset and the testing set of data was used to validate the model. The developed model (STTE) was then used to estimate the effect of starch doping, nano-silicon carbide, and preparation condition on T_C of MgB_2 superconductors and the obtained values are compared with the experimental results.

3.3. Optimization Strategy. The optimization strategy employed during the development of STTE was the test-set cross validation technique. In this case, the values of correlation coefficient, root mean square error, and mean absolute error were monitored in every run of the training and testing dataset for a group of parameters (regularization factor, kernel option, epsilon, and hyperparameter). In the course of searching through all the possible values of the parameters in a given range, the best performance measures were identified with the corresponding values of parameters for the fixed set of features. The whole process involves searching for the initial kernel option from the pool of the available kernel options and the identification of the best values of the parameter C and ϵ so as to identify the corresponding performance measures. The best values of the hyperparameters were further used to train SVR model. The values of hyperparameters that ensure optimum performance of the model are presented in Table 3.

4. Results and Discussion

4.1. Development of the Model (STTE). The STTE was developed using randomly selected ten experimental values of room temperature resistivity with their corresponding T_C . Excellent correlation coefficient of 100% was obtained in the

TABLE 3: Optimum parameters for the developed model (STTE).

SVR hyperparameter	Optimum value
C	10
Lambda	$e - 7$
Epsilon	0.2
Kernel option	0.8
Kernel function	Polynomial

TABLE 4: Comparison between the experimental and estimated value of T_C during the course of developing STTE.

Resistivity at room temperature ($\mu\Omega\text{-cm}$)	Experimental T_C (K)	Estimated T_C (K)	Percentage error (%)
Training phase			
17.000	38.90	39.03	-0.32
35.00	38.80	38.20	1.31
29.250	35.70	38.74	-8.50
9.600	39.40	39.20	0.51
17.992	38.50	38.72	-0.58
48.00	38.80	38.60	0.52
27.500	39.20	38.78	1.08
45.684	34.50	38.35	-11.15
Testing phase			
29.800	38.50	39.00	-1.30
7.800	41.00	39.24	4.29

course of testing the developed model prior to its usage. Low values of 1.29 and 0.279 for the root means square and mean absolute errors were, respectively, recorded. The pairwise comparison of the experimentally reported T_C and estimated values is depicted in Figure 1.

The actual (experimental value) and estimated values of T_C obtained during the development stage of STTE are presented in Table 4. The percentage errors were also calculated in order to observe the percentage deviation of the estimated values.

4.2. Application of the Developed Model (STTE) in Estimating T_C Disordered MgB_2 Superconductors. The developed STTE was used to estimate T_C of different disordered MgB_2 superconductors and the obtained values are compared with the experimental data. The utilization of the developed model involves feeding the model with the value of the room temperature resistivity and the model employs this value to generate the corresponding T_C .

4.2.1. Effect of Starch Doping on T_C of MgB_2 Superconductor Using the Developed Model. Addition of starch to MgB_2 superconductor alters its transition temperature as reported in the literature [4]. In order to assess the estimation strength of the developed model, the model was used to estimate the effect of starch doping on T_C of MgB_2 superconductor and the results are compared with the experimental values. Figure 3 shows the reduction in the transition temperature of MgB_2 superconductor when 1% concentration of starch was added.

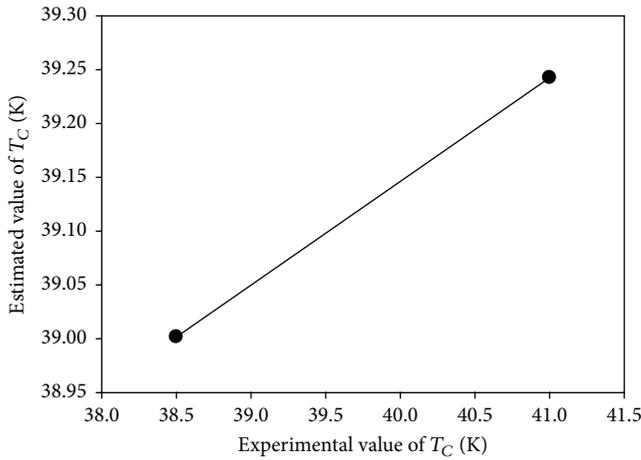


FIGURE 1: Correlation between the experimental and estimated value of T_C during the testing phase of STTE.

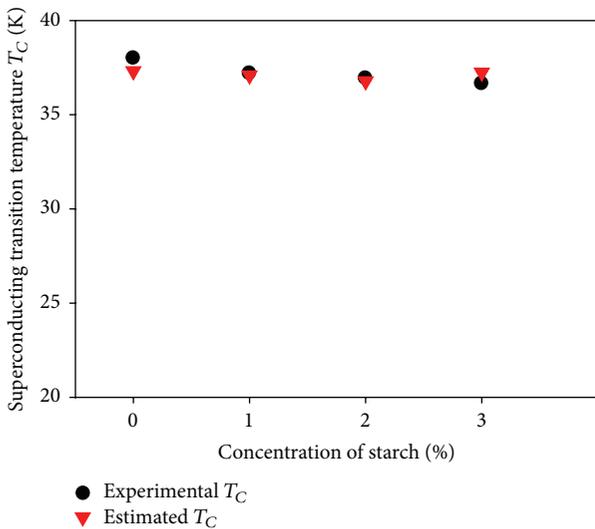


FIGURE 2: Effect of starch on T_C of MgB_2 superconductor using the developed model.

The transition temperature further reduced upon increase in the concentration of starch. The estimated results agree excellently with the experimentally reported values [4] (see Figure 2).

4.2.2. Effect of Nano-Silicon Carbide and Graphene on T_C of MgB_2 Superconductor Using the Developed Model. The effect of nano-silicon carbide (nano-SiC) and graphene on T_C of MgB_2 superconductor is also investigated and presented in Figure 3. The results of the developed model also agree well with the experimental values [39]. Introduction of graphene to MgB_2 already doped with 5% nano-SiC has little effect on T_C as depicted in Figure 3.

4.2.3. Effect of Preparation Condition (Heating Rate) on T_C of MgB_2 Superconductor Using the Developed Model. In order to further justify the effectiveness of the developed model, the effect of preparation condition on T_C of MgB_2

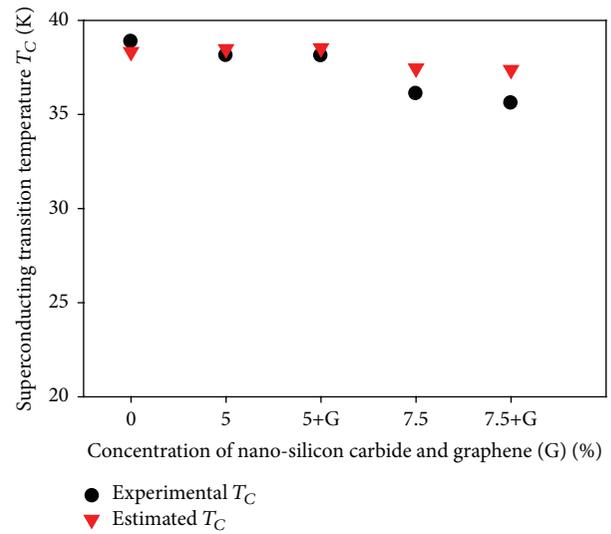


FIGURE 3: Effect of nano-silicon carbide and graphene on T_C of MgB_2 superconductor using the developed model.

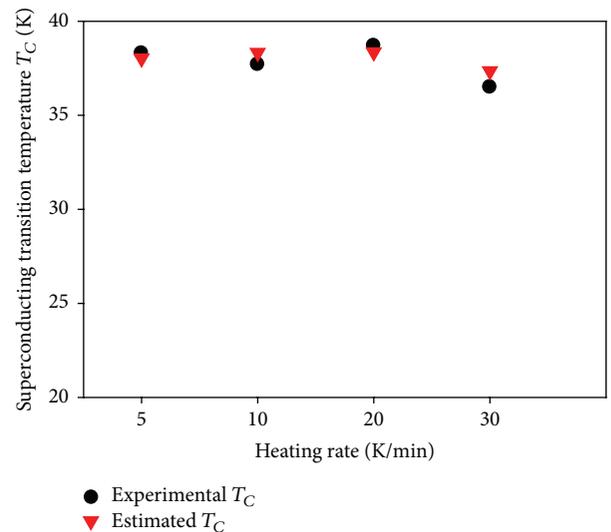


FIGURE 4: Effect of heating rate on T_C of MgB_2 superconductor using the developed model.

superconductor was estimated and presented in Figure 4. The rate of heating has significant effect on reducing T_C of MgB_2 superconductor, especially, when the rate was increased to 30 K/min as depicted in the graph. The results of the developed model show good agreement with the reported experimental values [40].

5. Conclusion and Recommendation

SVR was used to develop STTE through training and testing using test-set cross validation optimization technique with the aid of ten experimental values of room temperature resistivity and their corresponding T_C . The developed model (STTE) was then used to estimate the effect of starch doping, nano-silicon carbide, graphene, and preparation condition

on T_C of MgB_2 superconductors and the obtained values are compared with the experimental results. High accuracy obtained in the estimated T_C suggests that the developed model is capable of estimating T_C of disordered MgB_2 superconductors with slight deviation from the experimental values. The developed model is therefore recommended for quick estimation of T_C of disordered MgB_2 superconductors and can as well be incorporated into resistivity measuring instrument for direct estimation of T_C of disordered MgB_2 superconductors.

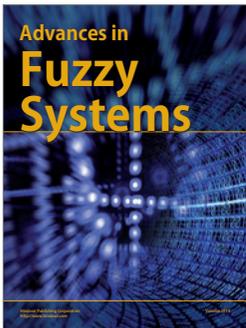
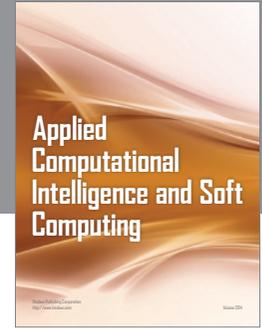
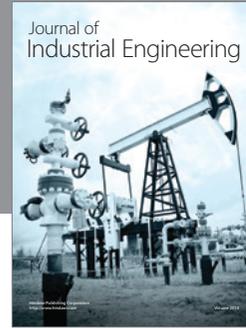
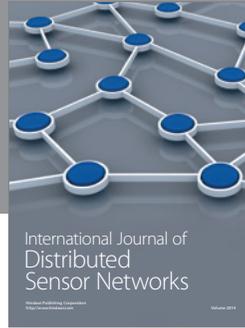
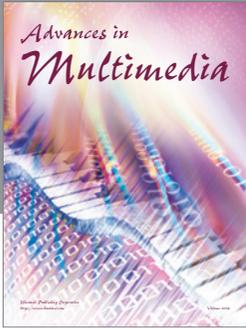
Competing Interests

The authors declare that they have no competing interests.

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