Development of Hybrid Gravitational Search Algorithm Based Support Vector Regression for Predicting Magnetic Ordering Temperature of Manganite using Ionic Radii Descriptors

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Abstract

Unique characteristic features of Magnetic Refrigeration Technology (MRT) which include environmental friendliness and better efficiency have promoted the chance of replacing the conventional Compression Gas System of Refrigeration (CGSR). One of the main challenges associated with practical implementation of MRT is the tuning of its magnetic ordering temperature (T_C) to ambient value. The present work utilizes the ionic radii as potential descriptors to develop hybrid Support Vector Regression (SVR) and Gravitational Search Algorithms (GSA) based model for estimating magnetic ordering temperature. The outcomes of the proposed method agreed closely with the experimental values. With the outstanding performance of the proposed hybrid SVR-GSA model, the magnetic ordering temperature of manganite (which serves as the refrigerant) can be easily tuned to the ambient value while dependency on ozone-depleting CGSR can be minimized.

Keywords: Manganite, Hybrid model, Curie temperature, Ionic radii

1.0 Introduction

Daily increase in the need for refrigeration calls for efficient and pollutant free technology that can replace the conventional compression gas system of refrigeration (CGSR) that is known to be harmful to the environment [1–3]. The uniqueness of magnetic refrigeration technology (MRT) includes high efficiency, low cost and environmental friendliness which makes it a reliable technology that can conveniently replace CGSR. The working principle of MRT is based on magnetocaloric effect which measures the response of magnetic material to varying magnetic field [4,5]. When magnetic material or magnetic refrigerant is in the vicinity of external magnetic field, the electronic spins of the magnetic refrigerant align along the axis of externally applied field and causes a reduction in the entropy of the system [6]. The resulting response of the electronic spins to the field sets the atoms present in the magnetic refrigerant into vibration and causes the thermal energy of the system to increase [7].

Magnetic ordering temperature (T_C) refers to the temperature at which the thermal energy becomes large enough to destroy the material macroscopic magnetic ordering. The random orientation of the electronic spins is restored upon removal of magnetic field and atomic vibration is therefore lowered due to increase in the entropy while the temperature of the system also reduced [5]. The change in the thermal energy of the system due to applied field results into magnetic refrigeration action. Implementation of this technology requires magnetic refrigerant with T_C around ambient value. Manganite based material stands a good chance of being used as magnetic refrigerant because it exhibits high magnetocaloric effect coupled with tunable T_C through doping mechanism [8–10]. Experimental determination of the nature and concentration of appropriate dopants is intensive and challenging.

Gravitational Search Algorithm (GSA) is a class of heuristic algorithm that is based on gravitational law and equation of motion and has been deployed in several applications [11–13]. It considers object in Newtonian description as agents with randomly assigned masses. Each agent is specified with position, velocity, acceleration and inertial mass. Effective gravitational force results into global movement of the agents towards those agents with heavier mass.

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Support vector regression (SVR) is a robust machine learning tool that has enjoyed a wide range of application due to its unique features which include non-convergence to local minimum as well as generalization of error bond. Its application extends to surface sciences [14–18], superconductivity [19–21] and petroleum industries among others [22–24] . It handles nonlinear problem using non-linear mapping function in transforming the data to high dimensional feature space where linear regression is constructed. SVR hyper-parameters have significant effect on the model performance and proper selection of these parameters ensure robust and efficient model. In the present work, a novel gravitational search algorithm (GSA) is used for hyper-parameters optimization.

Hybridization of this optimization method with SVR results into effective model for tuning T_C of manganite based materials. Implementation of the proposed model will definitely promote room temperature magnetic refrigeration and reduce dependence on ozone depleting system of refrigeration. The aim of this present work is to develop GSA-SVR model through which the T_C of manganite based material can be tuned using ionic radii descriptors which can be easily determined.

2.0 Materials and Methods

2. 1 Description of Dataset

Computational development of the proposed GSA-SVR model involves thirty seven (37) experimental magnetic ordering temperatures of manganite doped with wide varieties of metals as well as the ionic radii and concentration of dopants. Experimental magnetic ordering temperatures were obtained from previous studies [7, 25–30]. The formula for the manganite based materials that the proposed model works for is presented in equation (1).

$$A_{1-x-y} B_x C_y Mn_{1-z} D_z O_3 \tag{1}$$

Where
A represents rare earth cation
B represents alkali metal (or alkaline earth cation)
C and D represent doping materials

The chemical formula of manganite presented in equation (1) allows wide range of manganite based materials to be tuned for room temperature magnetic ordering and incorporate inherent robustness to the proposed model. The descriptors to the model are the ionic radii of the metals and their corresponding concentrations. Zero ionic radii and concentration are assigned to manganite that lack any of the components indicated in equation (1). For instance, manganite based material of $La_{0.7}Sr_{0.3}Mn_{0.9}Cr_{0.1}O_3$ chemical formula has descriptors which include the ionic radius of La (A=La), ionic radius of Sr (B=Sr), zero ionic radius for C and ionic radius of Cr (D=Cr). The concentrations are also included as 0.7, 0.3, 0 and 0.1 respectively. The concentration of the parent manganite is 0.9.

The data generated from statistical analysis of the dataset used in building the model are presented in Table 1. Useful insights about the dataset are contained in the mean, maximum, minimum and standard deviation presented in the table. Disparities in the dataset can also be inferred from the standard deviation. The correlation between each pair of the descriptors and the target are also presented. Correlation measures the degree of the linear relationship between the descriptors and the target. Many descriptors are characterized with relatively low correlation coefficient which is a strong indication that linear modeling technique cannot effectively handle this problem. Hence, a novel computational intelligence method that uses kernel function for transforming data into high dimensional feature space is proposed. The choice of SVR is due to its excellent generalization and predictive ability in the presence of limited number of data-points [19].

2.2 Computational Implementation of GSA-SVR Model

Computational development and implementation of GSA-SVR model was carried out within MATLAB computing environment. The ionic radii descriptors and the corresponding magnetic ordering temperatures were randomized and partitioned into training and testing set in the ratio of 8:2 respectively. The training dataset was used to build the model using GSA for hyper-parameter optimization while the generalization ability of the developed model was validated using testing set of data through test-set cross validation method [19,31]. The details of the computational description of GSA-SVR model are contained in Fig. 1. The optimum SVR hyper-parameters are presented in Table 2.

Table 1: Results of the Statistical Analysis carried out on the Dataset

	Radius of A (pm)	Conc. A	Radius of B (pm)	Conc. B	Radius of C (pm)	Conc. C	Radius of D (pm)	Conc. D	T_C (K)
Mean	114.70	0.64	121.70	0.24	62.68	0.12	51.41	0.05	204.87
Maximum	117.20	0.70	149.00	0.40	149.00	0.45	100.00	0.30	370.00
Minimum	109.80	0.15	113.00	0.10	0.00	0.00	0.00	0.00	80.00
Standard deviation	2.65	0.13	10.89	0.09	65.78	0.16	45.64	0.06	95.78
Correlation coefficient	49.07	-1.40	70.98	8.22	7.71	-3.39	-57.08	-41.11	

*Conc. A, B, C and D means concentration of dopants A, B, C and D

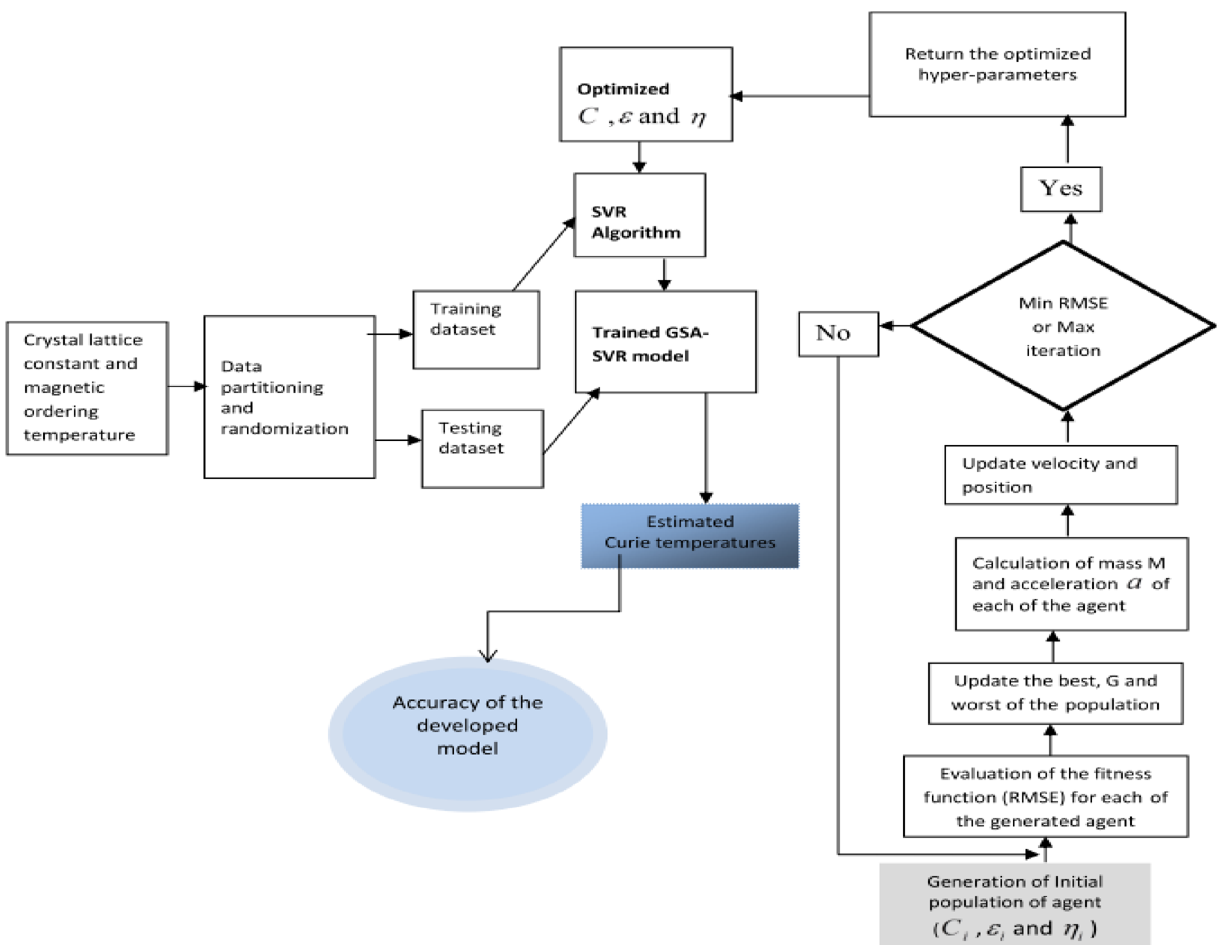

Fig. 1: Computational Flow Chart of the Proposed Model

Table 2: SVR Hyper-Parameters with Corresponding Optima Values

Hyper-parameter	Optimum value
Regularization factor	958.4912
Lambda	E-7
Epsilon	0.3596
Kernel option	0.9962
Kernel function	Gaussian function
Number of agents	20

3.0 Results and Discussion

3.1 Development of GSA-SVR

The correlation cross-plot obtained during the development of GSA-SVR model for tuning the T_C of manganite towards ambient value is presented in Fig. 2. Both training and testing datasets show high degree of correlation coefficient (CC). Presence of insignificant disparities between the estimated and experimentally reported T_C can also be deduced from alignment of the data-points shown in the figure. Low root mean square error (RMSE) and mean absolute error (MAE) were also obtained for the training and testing set of data (Table 3). The Table also highlighted measures of generalization and predictive ability of the developed model.

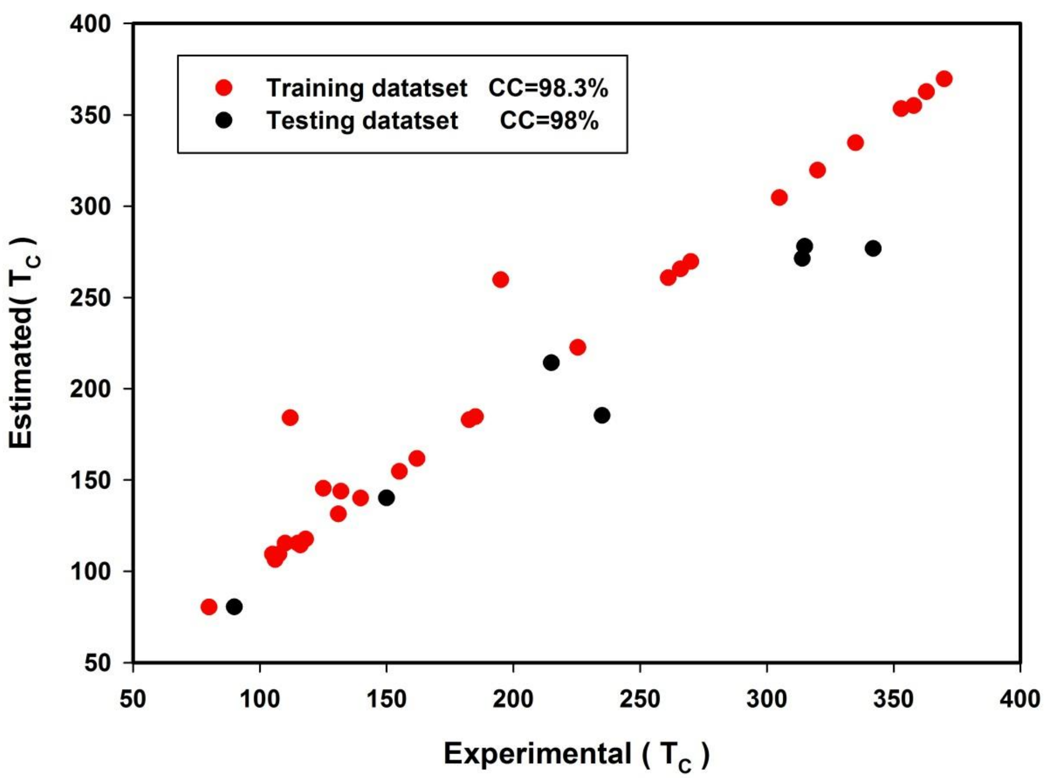

Fig.2:Correlation cross-plot between the experimental and estimated T_C

Table 3: Prediction Accuracy of the Developed SVR Model

	Training dataset	Testing dataset
CC (%)	98.3	98.0
RMSE (K)	18.26	38.02
MAE (K)	6.54	30.70

3.2 Investigating the Effect of Selected Metals on Magnetic Ordering Temperature (T_C) of Manganite

The effect of barium (Ba), lead (Pb) and strontium (Sr) on T_C of manganite using the developed model is presented in Fig. 3. Substitution of strontium with barium lowers the T_C from 370K to 335K. Also lead shifts the T_C to higher value as compared to the effect of barium. The estimated T_C conforms excellently with the experimentally reported values [32]. By using the developed model, the effect of different metals as well as their concentrations can be investigated with the aim of identifying a dopant that shift the T_C to desired value.

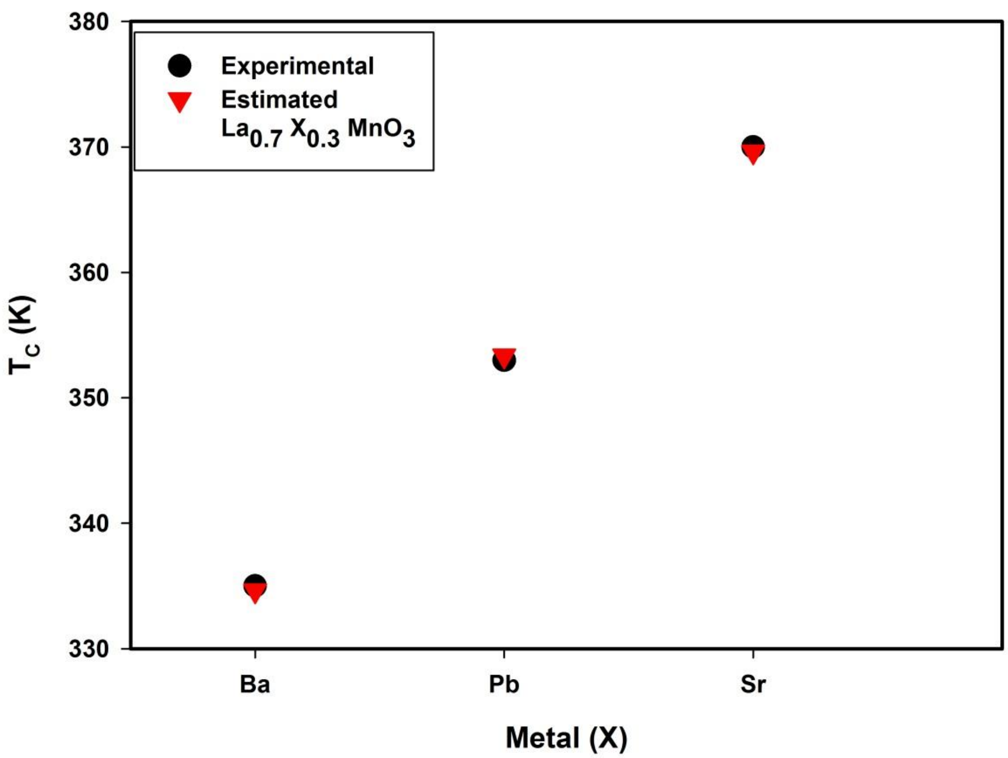

Fig.3:Effect of selected metals on manetic ordering temperature of $La_{0.7}X_{0.3}MnO_3$

4.0 Conclusion and Recommendation

This work hybridizes GSA with SVR for developing a robust model through which magnetic ordering temperature of manganite can be easily tuned around ambient value. The developed model is characterized with high correlation coefficient between the experimentally reported magnetic ordering temperatures and the estimated values. The developed GSA-SVR model has low RMSE of 38K. By implementing the proposed model, manganite with ambient T_C can be easily sought for and incorporated into refrigeration technology. This will lead to highly efficient system of refrigeration and a significant reduction in the use of ozone-depleting harmful conventional gas compression refrigeration.

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