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ORIGINAL PAPER

Predicting the Superconducting Transition Temperature T_c of BiPbSrCaCuOF Superconductors by Using Support Vector Regression

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Abstract According to an experimental data set on the superconducting transition temperature (T_c) of 21 BiPbSrCaCuOF superconductors under different process parameters including the amount of bismuth (n(Bi)), amount of oxygen (n(O)), sintering time (t) and sintering temperature (T), support vector regression (SVR) combined with particle swarm optimization (PSO) for its parameter optimization, was proposed to establish a model for prediction of the T_c of BiPbSrCaCuOF superconductors. The performance of SVR model was compared with that of back-propagation neural network (BPNN) and multivariable linear regression (MLR) model. The results show that the mean absolute error (*MAE*) and mean absolute percentage error (*MAPE*) of test samples achieved by SVR are smaller than those achieved by MLR or BPNN. This study suggests that SVR as a novel approach has a theoretical significance and potential practical value in development of high-T_c superconductor via guiding experiment.

Keywords BiPbSrCaCuOF · Superconducting transition temperature · Support vector regression · Regression analysis · Prediction

1 Introduction

Previous research shows that the zero-resistance transition temperature T_c of Bi-based superconducting material (Bi, Pb)$_2$Sr$_2$Ca$_2$Cu$_3$(OF)$_{10}$ is much higher than that of Y-based superconducting material, and it does not contain volatile toxic substances such as Tl_2O_3 when synthesizing, so that it is paid special attention by researchers. Up to now, there are many reports on the theoretical and experimental studies of BiPbSrCaCuOF superconductors [1–9] to investigate the influence of processing factors on the material properties. For the reason of complicated and time-consuming process, it is to synthesize materials and to determine T_c which may cause the waste of time and funds. In order to guide such experiment, Pan and Peng proposed a method to estimate the T_c of Bi-based superconductors sintered under different process parameters including bismuth doping level (n(Bi)), oxygen doping level (n(O)), sintering time (t) and sintering temperature (T) by using back-propagation neural network (BPNN) [9]. Motivated by the above Pan and Peng's work, we introduced a novel approach, i.e., the support vector regression (SVR) combined with particle swarm optimization (PSO) for its parameter optimization, integrating leave-one-out cross-validation (LOOCV), to predict the T_cs for 21 BiPbSrCaCuOF superconductors under different process parameters. The predictive results of SVR are also compared with those of BPNN and multivariable linear regression (MLR).

2 Methods and Materials

2.1 Theory of SVR

Support vector machine (SVM), proposed by Vapnik and co-workers in 1995, is based on structural risk minimization principle and statistical learning theory [10]. SVM has been successfully applied to solve classification and regression problems in many areas [11–17]. It is termed as SVR if SVM is served as a regressor. Owing to the well-known fact

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of that many real-world problems exhibit nonlinear characteristics, the basic idea of SVR, at first, is to map the input vectors $\boldsymbol{x}$ into a high-dimensional feature space $\boldsymbol{F}$ using a nonlinear mapping function $\Phi(\boldsymbol{x})$, and then to conduct a linear regression in space $\boldsymbol{F}$. Here, the vector $\boldsymbol{x}$ is the descriptor of a sample. The final regression function of SVR is as follows:

$$f(\boldsymbol{x}) = \sum_{i=1}^{l} (\alpha_i - \alpha_i^*) k(\boldsymbol{x}, \boldsymbol{x}_i) + b, \tag{1}$$

where, l is the number of support vectors, α_i and α_i^* are Lagrange multipliers, $k(\boldsymbol{x}, \boldsymbol{x_i}) = \Phi(\boldsymbol{x}) \bullet \Phi(\boldsymbol{x}_i)$ is a kernel function, b is a bias. In this study, the kernel function was adopted as a radial basis kernel, and it is formulated in (2). The detailed principle of SVR can be referred to Refs. [10] and [14].

$$k(\boldsymbol{x}, \boldsymbol{x}_i) = \exp\left(-\gamma \left\| \boldsymbol{x} - \boldsymbol{x}_i \right\|^2\right). \tag{2}$$

2.2 Choosing the SVR Parameters with PSO

The PSO method was proposed by Kennedy and Eberhart in 1995 [18]; it was motivated by social behavior of organisms, such as bird flocking and fish schooling. It is an optimization technique. The generalization ability of SVR relies entirely on three parameters, i.e., ε of the ε-insensitive loss function, the regularized constant C, and the kernel function parameter γ. Therefore, it is a key step to search the optimal parameters (ε, C, γ) for SVR. In this study, PSO was utilized to search the optimal parameters (ε, C, γ) of SVR [14]. Root mean square error (*RMSE*) is performed as the fitness function:

$$RMSE = \sqrt{\frac{1}{m} \sum_{i=1}^{m} (\hat{y}_i - y_i)^2}, \tag{3}$$

where, m denotes the number of training samples, y_i and $\hat{y}_i$ represent the measured (or target) values and estimated (or predicted) values for the ith training sample, respectively.

2.3 Data Set

The data set used in this study came from Ref. [9] and is listed in Table 1. This data set comprises 21 samples sintered under different conditions. In Table 1, n(Bi) means the amount of bismuth (n(Bi)), n(O) represents the amount of oxygen, t stands for sintering time and T is sintering temperature (T). In addition, the amount of lead (n(Pb)) and fluorine (n(F)) could be calculated by equations $n(\mathrm{Bi}) + n(\mathrm{Pb}) = 2$ and $n(\mathrm{O}) + n(\mathrm{F}) = 10$.

Table 1 Descriptors, measured T_cs and predicted T_cs by using MLR, BPNN and SVR for different samples

No.	n(Bi)	n(O)	t(h)	T	T_c (K)			
				(°C)	Exp.	BPNN [9]	MLR*	SVR
1	1.65	9.3	200	840	118	117.1	113.6	113.8
2	1.65	9.3	240	835	116	115.8	115.5	116
3	1.6	9.3	190	835	116	116.1	114.0	115
4	1.64	9.3	190	830	115	115.1	113.9	115.1
5	1.65	9	200	835	114	113.9	114.9	114
6	1.5	9	200	835	114	113.6	116.4	114
7	1.5	9.4	240	835	113	113	116.6	113
8	1.6	9.4	200	840	113	112.3	113.7	113
9	1.6	9.4	166	835	112	111.9	112.7	112
10	1.6	9.3	200	840	112	113.5	114.1	114.6
11	1.7	9.5	160	835	110	110	111.1	110
12	1.8	9.3	200	840	110	110.2	112.1	110
13	1.9	9.3	200	835	110	109.9	111.4	110
14	1.6	10	160	890	108	107.9	107.3	108
15	1.65	10	140	890	106	106.3	105.9	106
16	1.7	10	130	890	105	105.9	105.0	105
17	1.8	10	125	895	103	103	103.6	103
18	1.6	9.3	200	835	117	116.3	114.4	116.3
19	1.65	9.2	220	835	119	119.7	115.0	119
20**	1.65	8.6	240	835	120	119.5	117.8	119.5
21**	1.65	9.2	230	835	120	119.2	115.4	119.8

*MLR model $T_c = -9.9860n(\mathrm{Bi}) - 3.3775n(\mathrm{O}) + 0.0404t - 0.0570T + 201.3046$

**the test sample [9]

2.4 Evaluation of Model's Generalization Performance

Mean absolute error (*MAE*) and mean absolute percentage error (*MAPE*) are used for evaluate the performance of regression models. They are formulated respectively as the following:

$$MAE = \frac{1}{n} \sum_{i=1}^{n} \left| \hat{y}_i - y_i \right|, \tag{4}$$

$$MAPE = \frac{1}{n} \sum_{i=1}^{n} \left| \frac{\hat{y}_i - y_i}{y_i} \right|, \tag{5}$$

where, n denotes the number of test samples, y_i and $\hat{y}_i$ represent the measured (target) value and the predicted (estimated) value of the ith test sample.

3 Results and Discussion

The calculated T_cs by MLR, BPNN [9] and SVR are listed in Table 1. The pair-wise comparison of observed T_cs and predicted T_cs are displayed in Fig. 1.

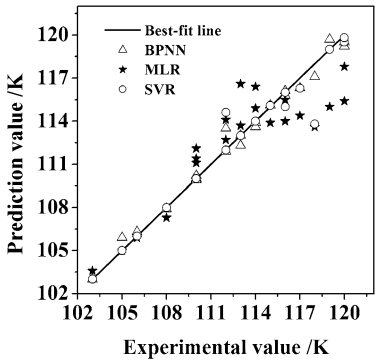

Fig. 1 Comparison of observed values vs. estimated values

Table 2 Comparison of prediction performance of different regression methods

Regression method	*MAE*/K		*MAPE*/%	
	Training	Test	Training	Test
BPNN	0.37	0.65	0.33	0.54
MLR	1.63	3.40	1.43	2.83
SVR	0.45	**0.35**	0.39	**0.29**

It can be seen from Fig. 1 that the vast majority of points (○) estimated by SVR lie on or very close to the best-fit line. But majority of points (★) estimated by MLR disperse on both sides of the line. From Table 1 and Fig. 1, it reflects that most values predicted by BPNN or SVR are in quite good agreement with the measured values and the prediction performances of BPNN and SVR are more effective than that of MLR.

Table 2 indicates that the test errors, *MAE* (0.35 K) and *MAPE* (0.29%) of SVR are smaller than those of BPNN or MLR, based on the same training set and test set. For SVR, either training *MAPE* or test *MAPE* is within an acceptable magnitude of 0.39%, which demonstrates that the SVR exhibits quite good prediction and generalization performance.

Figure 2 illustrates the effect of n(Bi) and n(O) on T_c predicted by SVR while as $t = 200$ h and $T = 835$°C, in which n(Bi) lies within the range of $1.4 \sim 2.0$ and n(O) within the range of $9.0 \sim 10.0$. It can be seen from Fig. 2 that, (i) the 3-D surface is similar to a saddle-like surface; (ii) the n(O)-T_c curve curvature to a convex shape, and the T_c would reach the maximum when n(O) is in the scope of $9.1 \sim 9.3$; (iii) the increase of T_c would benefit from the decrease of n(Bi). The above tendency is consistent with known experimental results [19, 20].

4 Conclusion

In this study, the model for predicting the T_c of the doping Bi-based superconductor under different synthesis conditions is set up by using SVR approach combined with PSO, and the prediction results are compared with those of BPNN and MLR models. The predicted error of SVR model is smaller than that of BPNN or MLR models for the identical test samples.

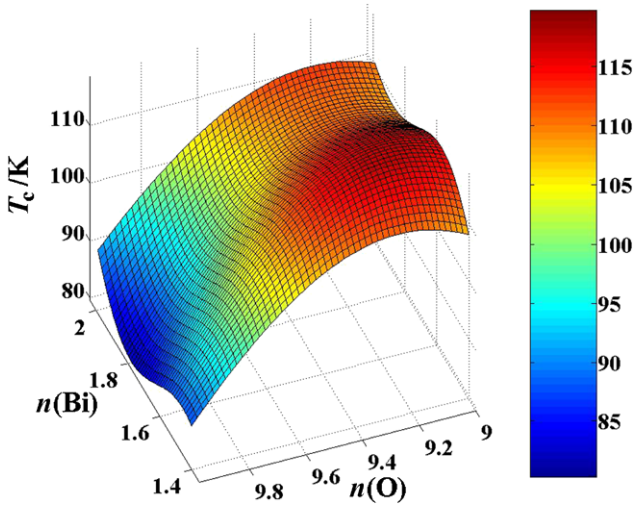

Fig. 2 Effect of n(Bi) and n(O) on T_c predicted by SVR ($t = 200$ h and $T = 835$°C)

On the other hand, the SVR prediction model can be used to forecast the T_c of superconductor under different process parameters accurately. These indicate that SVR as a novel approach has a theoretical significance and potential practical value in development of the high-T_c superconductor via guiding experiment.

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