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Performance Prediction of Magnetocaloric Materials Using CNN and SVR

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Abstract: *In this paper, a hybrid model CvBlock-SVR combining convolutional neural network (CNN) and support vector regression (SVR) is proposed for predicting the properties of magneto-thermal effect materials. The chemical composition descriptors are constructed by Magpie and the material features are augmented using a convolutional block (CvBlock), and the augmented features are subsequently modelled with SVR to accurately predict the transition temperature (T_{tr}) of the material. Training the pervasive CvBlock-SVR model on a dataset of all magneto-thermal effect materials achieved $R^2 = 0.871$ and MAE = 24.937 K for T_{tr} prediction.The model was also successfully applied to the prediction of materials space such as Gd-Al, Gd-Co-Al, and $Fe_{93-x-y}Zr_7B_xCu_y$, which verified its high accuracy and wide applicability. It is shown that the CvBlock-SVR model not only provides accurate prediction results, but also has wide applicability and is suitable to be applied to the prediction of the properties of different types of magneto-thermal effect materials.*

Keywords: *Magnetocaloric materials; Feature enhancement; Machine learning in materials science*

1. Introduction

Conventional vapor-compression refrigeration systems are inherently constrained by their bulky configurations, substantial weight, and suboptimal energy efficiency, coupled with the prevalent use of environmentally hazardous refrigerants that contribute to atmospheric degradation[1]. Among emerging alternative refrigeration technologies, magnetic refrigeration demonstrates significant promise. The performance of solid-state magnetocaloric materials is conventionally evaluated through the isothermal magnetic entropy change (ΔS), which quantifies the rate of order-disorder transition in magnetic moment systems[2]. The maximum magnetic entropy change (ΔS_M) occurs during magnetic phase transitions, making the critical magnetic phase transition temperature (T_{tr}) a crucial operational parameter. In most magnetocaloric materials, particularly ferromagnetic systems, the Curie temperature (T_C)—which marks the ferromagnetic-to-paramagnetic phase transition – serves as the critical transition temperature (T_{tr}). Magnetic refrigeration demonstrates operational versatility across distinct temperature ranges. Notably, within the cryogenic regime (20–120 K), it facilitates the efficient liquefaction of hydrogen, nitrogen, and helium[3], while in the near-ambient temperature range (270–320 K), emerging applications span domestic climate control and commercial food preservation. Despite the technology's first successful prototype demonstration four decades ago[4], it has yet to achieve widespread commercial implementation. A fundamental challenge stems from the current lack of commercially viable magnetocaloric materials[5]. This limitation is further compounded by the significant technical hurdles in engineering cost-effective, high-performance alternatives based on earth-abundant and non-toxic constituents[6]. Current material discovery predominantly relies on empirical trial-and-error approaches a time-intensive process requiring extensive domain expertise. Although high-throughput approaches such as first-principles calculations and thermodynamic models have been employed to predict magnetocaloric properties, these investigations remain highly complex, demanding detailed material specifications. Emerging machine learning (ML) techniques offer transformative potential for accelerating magnetocaloric material discovery. ML algorithms can autonomously extract meaningful patterns from experimental datasets, enabling data-driven decision-making for material design[7].

2. Data sets and descriptors

The magneto-thermal effect material dataset used in this study is extensively derived from the published literature[8]and includes 1606 magneto-thermal effect materials. This dataset covers the

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material types summarised by V. Franco et al[2], including La(Fe, Si/Al)$_{13}$, Heusler metals, Gd_5(Si, Ge)$_4$, manganites, amorphous materials and Laves phase compounds. A detailed analysis and visualisation of these magneto-thermal effect material data is presented in the next section. The magnetothermal effect materials collected in this study are mainly dominated by Mn, Fe, La and Co, and Gd. In the dataset, 729 materials contain the element Mn; more than 500 materials contain the elements Fe or La; and the elements Gd and Co are also the main research elements in the field of magneto-thermal effect. As ferromagnetic elements, Mn, Fe, and Co are widely present in magnetothermal effect materials, and they play a crucial role in the ferromagnetic to paramagnetic phase transition during the magnetothermal effect. In particular, Gd, as the only lanthanide metal with a Curie temperature close to room temperature, drives the research and development of room-temperature magnetocooled materials. It is noteworthy that, in addition to these elements, the magnetothermal effect properties can be modulated by other ions in the periodic table, which provides a potentially very wide scope for chemical exploration in the design of new magnetothermal effect materials.

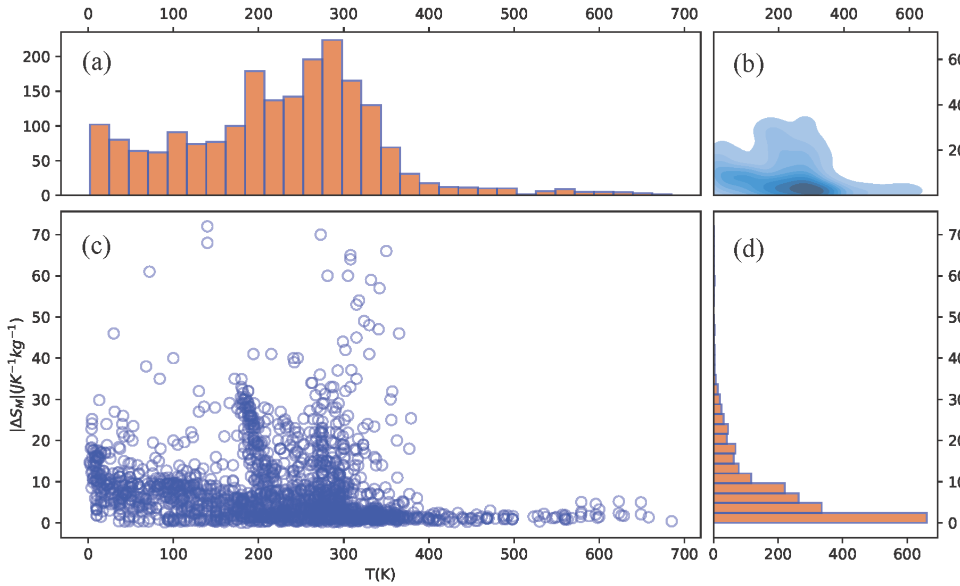

Figure 1 Visualisation of T_{tr} and ΔS_M distributions for magnetothermal effect materials. (a) Histogram of Ttr distribution; (b) Density plot of T_{tr} and ΔS_M distribution; (c) Scatter plot of T_{tr} and ΔS_M; (d) Histogram of ΔSM distribution

Figure 1 illustrates the distribution of ΔS_M and T_{tr} for the 1606 magnetothermally effected materials in this study.The distribution of T_{tr} spans the temperature range of 2.0-685 K, as shown in Figure 1(a). In the dataset, $Tm_{39}Ce_{16}Co_{20}Al_{25}$ and $Tm_{39}Pr_{16}Co_{20}Al_{25}$[9] have the smallest T_{tr} values, both of which are 2 K. $FeCoNi_{0.5}Cr_{0.5}Al$ has a T_{tr} of 685 K [10], which is the largest T_{tr} value used in this study.

Material data distribution imbalance is inevitable and has a significant impact on model performance. In the model training, this study will use the orthogonal distribution to handle the training data. In the dataset, the T_{tr} of the same magneto-thermal effect material is reported by different studies for multiple values, which vary to different degrees. This requires us to clean the data for better training of the model. Samples with T_{tr} values deviating by more than 50 K are also eliminated in this paper and the median is taken for the remaining samples with multiple T_{tr} values. Finally, 1576 materials were used for the T_{tr} prediction study.

Digitisation of materials is the most important component of the machine learning paradigm. The experimental dataset used in this study covers a wide range of magneto-thermal effect material types, and therefore, the use of universal compositional features as material descriptors is the most appropriate choice. The advantage is that the properties of unknown magneto-thermal effect materials can be predicted based on chemical formulae alone[11]. However, due to the lack of other features such as structure, some isomers will no longer be considered in this study. In addition, the lack of structural information of the materials makes model training a great challenge and therefore more examples are needed to support the training of the models[12]. Therefore, this study did not focus on a single type of magneto-thermal effect material, but trained a generic performance prediction model using the entire dataset. In the prediction task of T_{tr}, component features were constructed using Magpie.

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3. Modelling framework

In this paper, CNN is used as a feature extractor for the magnetothermal effect material, and the extracted features are subsequently used as inputs to the SVR prediction model to predict the ΔS_M and T_{tr} of the magnetothermal effect material, and the model framework is shown in Fig. 2. The model in the figure includes CvBlock and Fully Connected Network (FC) and SVR, and of course the embedding layer for input vector processing. FC exists to train the CvBlock, denoted as CvBlock-FC model. SVR exists to predict the T_{tr} of the material based on the CvBlock output, denoted as the CvBlock-SVR model. The framework of these main models is described in detail below.

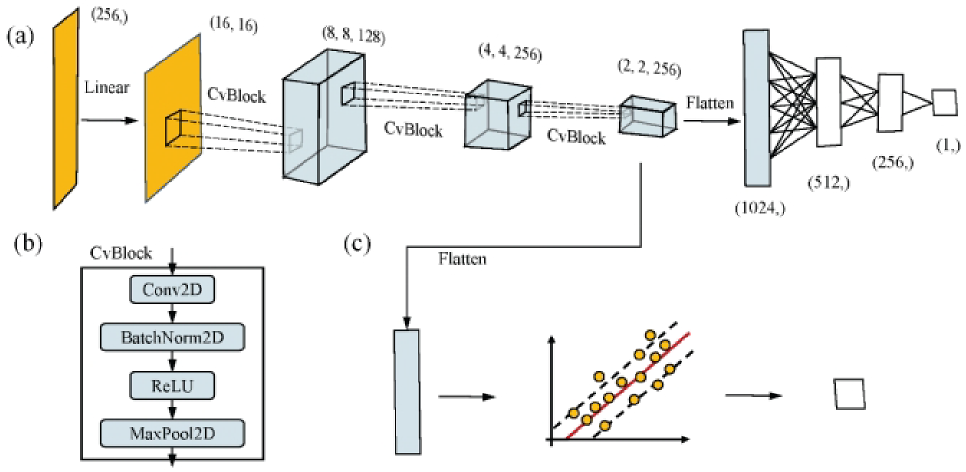

Fig. 2 Framework for predicting the properties of magneto-thermal effect materials. (a) CNN prediction of magneto-thermal properties, including embedding layer, three convolutional modules and three hidden layers of fully connected network; (b) convolutional modules, including 2D convolution, batch normalisation, ReLU activation function, and 2D max-pooling; (c) SVR prediction of magneto-thermal properties, using the CNN output features as inputs to the model

3.1 Embedding layer

One-dimensional vectors cannot be directly input into CvBlock, they need to be transformed into two-dimensional shapes. The method of Nam C[13] is to reshape the descriptors into two-dimensional matrices as CNN inputs, but there are obvious shortcomings in this method. The basic principle of CNN is to update the current feature values by the values of the features and their surrounding neighbours, and if the one-dimensional descriptor vectors are directly reshaped into two-dimensional matrices, this is equivalent to artificially defining the neighbourhood relationship between features, which is inconsistent with the unknown nature of the relationship between features in physics.

To solve this problem, an embedding layer is introduced in this paper. Through a learnable embedding layer, the 145-dimensional descriptor vectors are mapped to 256 dimensions and further reshaped into a 16 × 16 2D matrix. This embedding layer is implemented by a linear transformation, i.e., and denote the input 145-dimensional vectors and the output 256-dimensional vectors, respectively, and and are both learnable parameters. The advantage of this method is that it avoids the need to artificially set the adjacencies between the features and makes it more suitable for the task of nonlinear prediction of the performance of the magneto-thermal effect by mapping the features to higher dimensions.

3.2 Convolutional Block

The output of the embedding layer is a 16 × 16 matrix representing a single channel with a size of 16 × 16. Next, the feature matrix is processed through three CvBlocks. Each CvBlock consists of the following layers: a 2D convolutional layer (Conv2D), a batch normalisation layer (BatchNorm2D), a rectified linear unit function activation function layer (ReLU), and a 2D maximal pooling layer (MaxPool2D).

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3.3 Fully Connected Neural Networks (FC)

Fully-connected neural networks are only used for model training and are not involved in model prediction tasks. The output of the CvBlock module is the feature matrix, but these matrix features are not directly understandable, let alone defining a standard matrix labelling for training CvBlock networks. Therefore, in this paper, a fully connected layer is added after the CvBlock module in order to train the convolutional neural network efficiently.

3.4 Support Vector Regression (SVR)

In order to improve the prediction accuracy of the magneto-thermal properties, the fusion model CvBlock-SVR is proposed in this paper. the model adopts SVR to predict the properties of the magneto-thermal effect materials based on the features extracted by CvBlock.

4. Model training and performance

In this paper, a convolutional neural network is used as a feature extraction tool for magneto-thermal effect materials and SVR is used to predict the T_{tr} of magneto-thermal effect materials based on this feature, the training and performance of the model is discussed below.

4.1 Forecast of T_{tr}

Prediction of T_{tr} for magneto-thermal effect materials using CvBlock-SVR.

4.2 CvBlock training and results

In the T_{tr} task of predicting magneto-thermal effect materials, in this paper, the dataset is divided into training and test sets in the ratio of 9:1, and the training set is further divided into training data and validation data in the ratio of 8:2. In the study, Mean Square Error (MSE) is used as the loss function and AdamW is used as the network parameter updating strategy, while the callback function ReduceLROnPlateau is used to dynamically adjust the learning rate. All experiments were implemented in Python environment based on Pytorch.

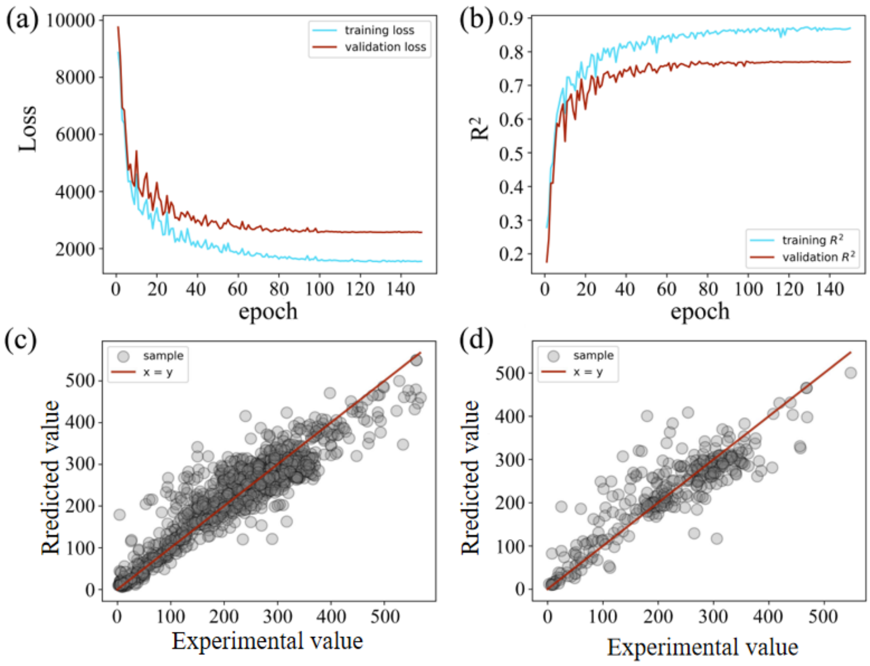

Figure 3 Variation of (a) loss MSE and (b) R^2 with the number of training rounds (epoch) for the training process of the CvBlock-FC model in the T_{tr} prediction task. The blue curve indicates the variation on the training set and the red curve indicates the variation on the validation set. (c) Predictive performance of the model on the training set; (d) Predictive performance of the model on the test set

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CvBlock-FC was trained 150 times on the training set, and the changes in MSE and R^2 are shown in Figure 3(a)(b). The convergence point of the model on the training data is $R^2 = 0.869$ and MSE = 1551.01 K as shown in Fig. 3(a); on the validation data, it converges to $R^2 = 0.769$ and MSE = 2567.34 K as shown in Fig. 3(b). As can be seen from the figure, the improvement of the training process plateaus after 100 sessions, at which point the model performance on the training and validation data is $R^2 = 0.867$, MSE = 1581.80 K and $R^2 = 0.769$, MSE = 2577.73 K. Given the limited space for subsequent optimisation, this study stops the training after 150 sessions and evaluates the model performance on the test set, which results were $R^2 = 0.747$, MSE = 2647.81 K and MAE = 34.966 K. The test results of the model are visualised in Fig. 3(c)(d): Fig. 3(c) shows the performance on the training set, with the experimental values in the horizontal and the predicted values in the vertical coordinates; and Fig. 3(d) shows the performance on the test set. It can be seen that the model predicts most of the magneto-thermal effect materials T_{tr} in the 200-400 K interval more satisfactorily.

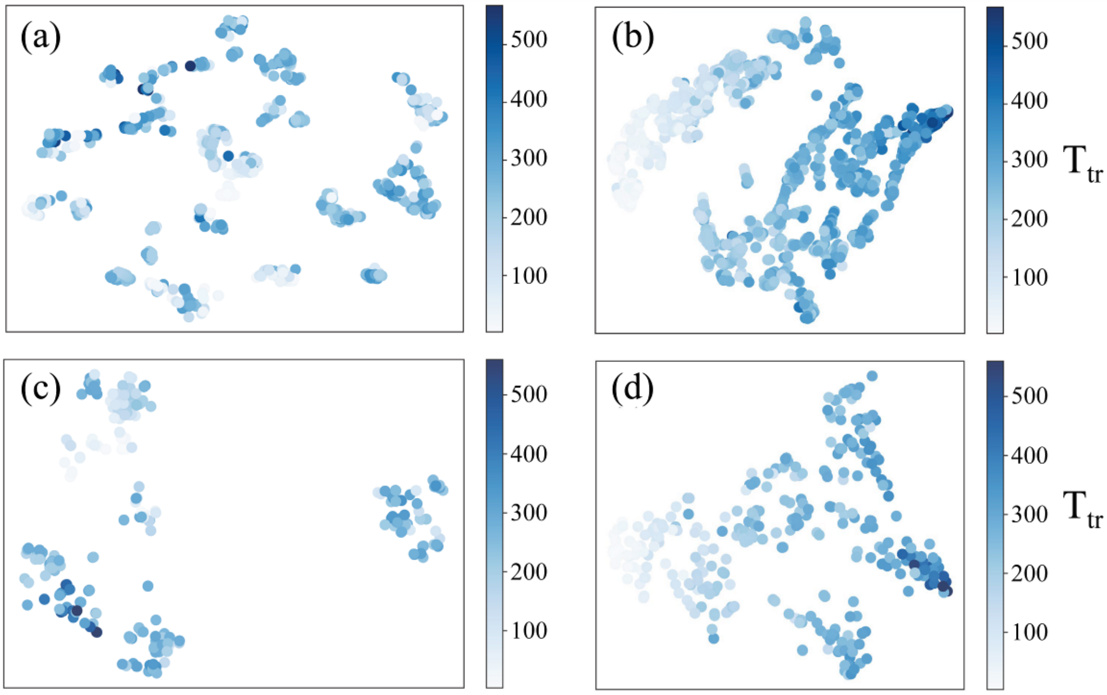

Fig. 4 Spatial distribution of t-SNE features of magneto-thermal effect material descriptors with respect to T_{tr}. On the training set (a) 2D visualisation of t-SNE based on Magpie features and (b) t-SNE visualisation based on 1024-dimensional feature vectors output by CvBlock. On the test set (c) t-SNE visualisation based on Magpie features and (d) t-SNE visualisation based on 1024-dimensional feature vectors output by CvBlock. The colour bar indicates the size of the T_{tr}

In order to further evaluate the descriptor processing capability of CvBlock, in this study, the initial Magpie features of the magneto-thermal effect material and the features after CvBlock processing are downscaled and visualised by t-SNE, respectively. Figures 4(a)(b) and 4(c)(d) show the visualisation results for the training and test sets. Figure 4(a) and Figure 4(b) show the distribution of the training set based on Magpie features and CvBlock features, respectively, where the colour shade of the scatter indicates the size of T_{tr}. As can be seen from the figures, the distribution of Magpie features is more chaotic, while CvBlock features are able to clearly distinguish materials with different T_{tr} values. Importantly, Figure 4(c)(d) shows the visualisation results of the test set, where the CvBlock features exhibit better differentiation compared to the Magpie features. This demonstrates the superiority of CvBlock in terms of feature extraction and generalisation capabilities.

5. Conclusion

In this study, a method CvBlock-SVR combining *CNN* and SVR is proposed for predicting the properties of magneto-thermal effect materials. The model achieves accurate prediction of the properties of magneto-thermal effect materials by using the chemical composition as a descriptor of the material, augmenting the descriptor using a convolutional block (CvBlock), and modelling the augmented feature vectors in combination with SVR. A generic CvBlock-SVR model was trained on all magneto-thermal

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effect materials to predict the T_{tr} of the materials.The experimental results show that the model achieves an R^2 of 0.871 in T_{tr} prediction and an MAE of 24.937 K. These results fully demonstrate the excellent ability of the CvBlock-SVR model in capturing the performance characteristics of the materials, which significantly improves the prediction accuracy.

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