

Bridging Chemically Distinct Coating Systems: Cross-System Transfer Learning Enables Discovery of Ultralow-Thermal-Conductivity Ferroelastic Tantalates

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Bridging Chemically Distinct Coating Systems: Cross-System Transfer Learning Enables Discovery of Ultralow-Thermal-Conductivity Ferroelastic Tantalates

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Abstract

Two ferroelastic rare-earth tantalate ceramics with ultralow thermal conductivity are discovered via cross-system transfer learning, achieved by transferring knowledge from chemically distinct oxide systems to the data-scarce RETaO₄ domain. Virtual screening of over 300,000 multicomponent candidates identified two previously unexplored ferroelastic compositions, Y_{0.40}Ce_{0.10}Sm_{0.30}Gd_{0.10}Er_{0.10}TaO₄ and Y_{0.30}Ce_{0.10}Sm_{0.10}Eu_{0.10}Gd_{0.10}Dy_{0.10}Ho_{0.10}Yb_{0.10}TaO₄, which achieve ultralow thermal conductivities of 1.276 and 1.307 W·m⁻¹·K⁻¹ at 900 °C, respectively; the former is the lowest thermal conductivity reported to date for bulk RETaO₄ ceramics at this temperature. Feature analysis reveals that two physically interpretable descriptors, effective nuclear charge and ionic bond strength, govern the prediction by capturing phonon group velocity and phonon scattering, respectively. First-principles calculations,

phonon analysis, and electron microscopy demonstrate that lattice distortion and heterogeneous bonding induce phonon localization, while ferroelastic domains, dislocations, and point defects cooperatively suppress heat transport. This work establishes a generalizable paradigm coupling cross-system transfer learning with minimal physically interpretable descriptors for discovering compositionally complex ceramics under data scarcity.

Introduction

Thermal barrier coatings (TBCs) serve as crucial protective materials for aero-engines and gas turbines, playing an increasingly vital role in elevating the operating temperatures of hot-section components and extending their service life.^[1-4] Although yttria-stabilized zirconia (YSZ) remains the most widely used material, it undergoes phase transformation at higher temperatures (>1200 °C). This phase transformation can lead to small volume expansions, potentially causing material failure. Additionally, the thermal conductivity of YSZ at 1000 °C is $2.3 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$, which is still relatively high.^[5-8] As aero-engines and gas turbines continue to evolve toward higher temperatures and higher thrust-to-weight ratios, there is a pressing need to explore new TBC materials with low thermal conductivity.

Ferroelastic rare-earth tantalate (RETaO_4) is regarded as a highly promising TBCs material due to its low thermal conductivity, high coefficient of thermal expansion, and high-temperature phase stability.^[9-14] Based on the concept of high-entropy ceramics,^[15-18] multi-component rare-earth tantalates have garnered significant research interest owing to their unique structural characteristics and functional performance.^[19, 20] Wang et al.^[21] successfully synthesized $(10\text{RE}_{0.1})\text{TaO}_4$ through high-entropy engineering, demonstrating a remarkably low thermal conductivity of $1.32 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ at 900 °C. However, there are many kinds of elements involved in RE-site, and the combination of different element types and proportions constitute a complex and high-dimensional search space. Traditional trial-and-error methods are very time-consuming and costly. While the emergence of high-throughput computations based on density functional theory (DFT) computations have accelerated the search process to a certain extent, these methods still face challenges such as modeling difficulties and large consumption of computational resources.

In recent years, significant progress has been made in the development of artificial intelligence (AI) and materials informatics.^[22-26] Data-driven machine learning techniques have emerged as a viable approach in materials design, accelerating the design process by mining the relationship between material structure/composition and properties.^[27-32] Zhang et al.^[33] developed an intelligent design approach that efficiently screened $\text{A}_2\text{B}_2\text{O}_7$ -type high-entropy oxides (HEOs) with ultralow thermal conductivity by integrating domain knowledge-assisted data-driven machine learning strategies. They combined the XGBoost algorithm with high-throughput first-principles calculations to successfully predict the optimal composition $(\text{Sc}_{0.2}\text{Y}_{0.2}\text{La}_{0.2}\text{Ce}_{0.2}\text{Pr}_{0.2})_2\text{Zr}_2\text{O}_7$ with thermal conductivity as low as $1.59 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$

from 6,188 candidate $(5\text{RE}_{0.2})_2\text{Zr}_2\text{O}_7$ materials, achieving high agreement between experimental validation result and predicted values. Xia et al.^[34] developed an interpretable machine learning framework that integrates a four-step feature selection process with SHAP analysis. Using this method, they predicted the key thermophysical and mechanical properties of zirconia-based thermal barrier coatings, specifically thermal conductivity (TC), thermal expansion coefficient (TEC), and fracture toughness (K_{ic}). The results demonstrate that these models exhibit robust predictive performance: the R^2 values for TC and TEC both exceed 0.95, while the R^2 value for K_{ic} exceeds 0.92. Additionally, the models successfully identified the most influential atomic features governing these properties. However, in previous studies on thermal conductivity prediction, models were typically trained only on data from a single system. This approach not only suffers from limited sample size but also struggles to ensure the model's generalization capability across unknown systems. To address this challenge, transfer learning has emerged as a promising solution.^[35-38] This technique leverages existing large-scale datasets from different but physically similar material systems to enhance the prediction accuracy of target material thermal conductivity. The core idea of transfer learning is to first pre-train a model on the source domain (extensive data from related materials) and then transfer the learned feature representations to the target domain (a thermal conductivity system with limited data) via domain adaptation constraints or fine-tuning strategies, greatly enhancing the model's generalization ability on the target data.

In this work, to address the contradiction between complex compositional space and sparse small samples, we constructed a multi-system dataset by systematically compiling thermal conductivity data for various thermal barrier coating systems beyond RETaO_4 , including rare-earth niobates, zirconates, and cerates. These systems share identical rare-earth cations with RETaO_4 and exhibit similar phonon scattering mechanisms.^[39-42] Based on this multi-system dataset, we initially trained a deep neural network, which was then fine-tuned specifically for the RETaO_4 system using transfer learning strategies. Compared with the traditional machine learning model, the correlation coefficient R^2 improved from 0.832 to 0.909. Finally, we employed the transfer learning-optimized deep neural network model to predict the composition space of RETaO_4 (RE=Y, Ce, Nd, Sm, Eu, Gd, Dy~Lu) system, which consists of a virtual RETaO_4 composition space containing 300,564 candidate compositions, and quickly screened out multi-component rare-earth tantalate materials with lower thermal conductivity: $\text{Y}_{0.40}\text{Ce}_{0.10}\text{Sm}_{0.30}\text{Gd}_{0.10}\text{Er}_{0.10}\text{TaO}_4$ ($1.276 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ at 900°C), $\text{Y}_{0.40}\text{Ce}_{0.10}\text{Sm}_{0.20}\text{Eu}_{0.10}\text{Gd}_{0.10}\text{Dy}_{0.10}\text{TaO}_4$ ($1.470 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ at 900°C), $\text{Y}_{0.40}\text{Ce}_{0.10}\text{Sm}_{0.10}\text{Eu}_{0.10}\text{Gd}_{0.10}\text{Dy}_{0.10}\text{Yb}_{0.10}\text{TaO}_4$ ($1.341 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ at 900°C), and $\text{Y}_{0.30}\text{Ce}_{0.10}\text{Sm}_{0.10}\text{Eu}_{0.10}\text{Gd}_{0.10}\text{Dy}_{0.10}\text{Ho}_{0.10}\text{Yb}_{0.10}\text{TaO}_4$ ($1.307 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$ at 900°C). Meanwhile, the underlying mechanism for the low thermal conductivity was elucidated through TEM and computational analysis, providing new ideas for the design of multi-component rare-earth tantalate materials. The workflow of this study is shown in Fig. 1.

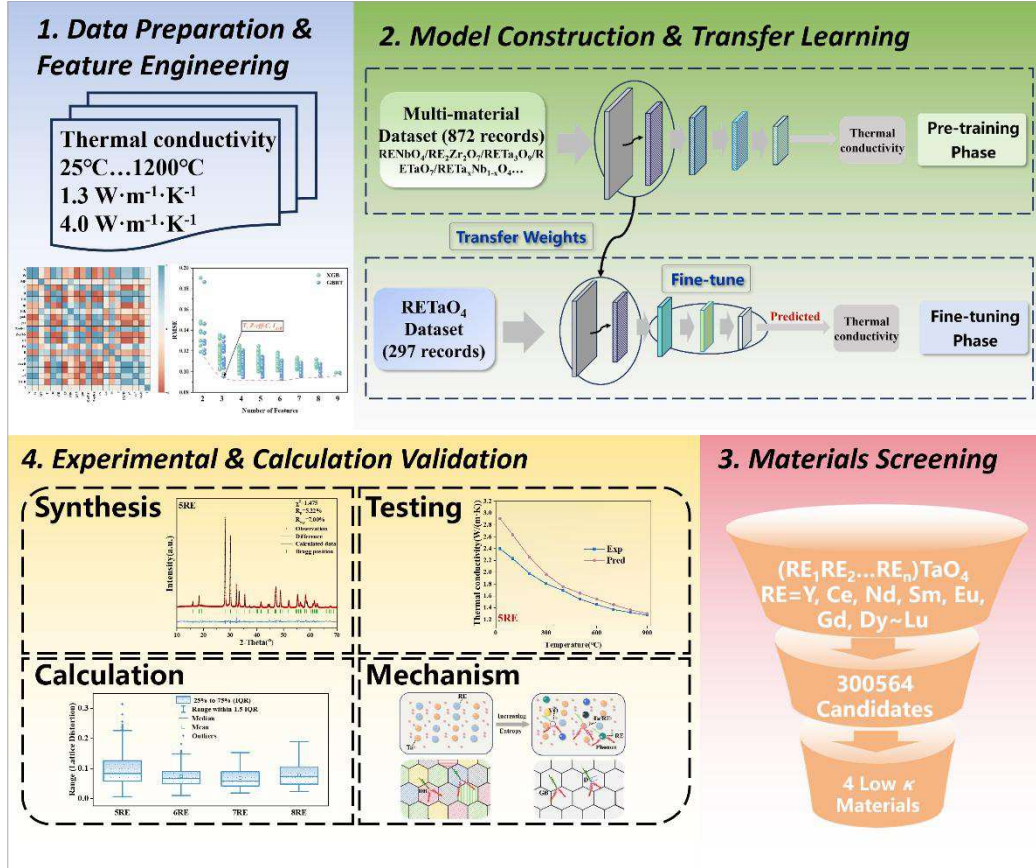


Figure 1. Workflow for Low Thermal Conductivity Multicomponent RETaO₄ via Transfer Learning

Results

Data preparation and feature engineering

In this work, a specialized dataset of thermal conductivity for rare-earth tantalates (RETaO₄) was constructed through systematic collection and rigorous screening. This dataset was compiled from published literature on rare-earth tantalate materials,^[12, 19, 21, 43-52] supplemented by unpublished experimental data from our research group. All data follow the general chemical formula RETaO₄, where RE denotes rare-earth elements, covering twelve species: Y, Ce, Nd, Sm, Eu, Gd, and Dy–Lu. This dataset covers single-, binary-, and multi-rare-earth compositions. To ensure consistency, only the thermal conductivity data corresponding to the monoclinic phase were included. Ultimately, a total of 297 thermal conductivity records were gathered for 31 RETaO₄ materials across the temperature range of 27 °C to 1200 °C, with values ranging from 1.32 W·m⁻¹·K⁻¹ to 3.97 W·m⁻¹·K⁻¹. This dataset encompasses systems from single-component to ten-component compositions. Fig. 2a displays the distribution of temperature and thermal conductivity in the dataset, while the distribution of components and elements can be

found in Supplementary Fig. S1.

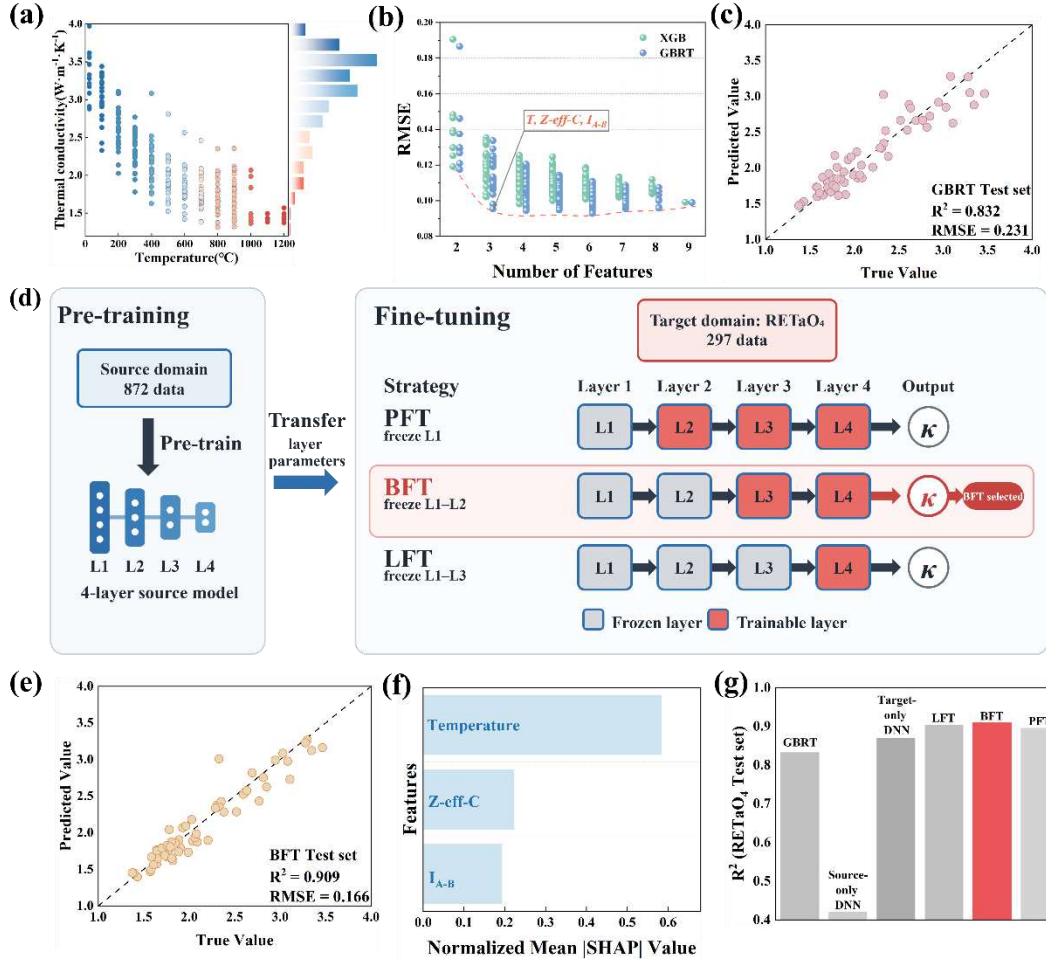


Figure 2. Feature selection, cross-system transfer learning, and model interpretation for predicting the thermal conductivity of RETaO₄. (a) Distribution of temperature and thermal conductivity for materials within the original RETaO₄ dataset. (b) Identification of the optimal feature subset. (c) Comparison between the predicted and experimental thermal conductivities for the independent test set using the GBRT model. (d) Schematic of the cross-system transfer-learning framework. (e) Comparison between the predicted and experimental thermal conductivities of the independent test set using the BFT model. (f) Feature importance of the BFT model quantified by the normalized mean absolute SHAP value. (g) Comparison of the test-set R^2 obtained using GBRT, source-only DNN, target-only DNN, LFT, BFT, and PFT models.

We established a composition-based physical feature framework that requires no complex DFT calculations, instead deriving features through simple mathematical operations on compositional data.^[28, 53-60] The feature descriptions and symbols are provided in Supplementary Table S1. Due to the high initial features dimension, directly training models using these features yields suboptimal results. Furthermore, highly correlated features often contain overlapping information, contributing little to the model's predictive performance. Feature dimensionality reduction is therefore crucial.

We first calculated the Pearson correlation coefficients between features and constructed a correlation matrix. We set ± 0.85 as the threshold, and features with coefficients greater than the threshold were grouped together (heatmap of feature correlations shown in Supplementary Fig. S2). Then, we selected a feature that has a physical association with the target attribute and can represent the other features in the group for retention (as shown in Supplementary Table S2). nine features were retained: Mass disorder parameter (m^*), radius disorder parameter (r^*), first ionization energy (FIE), ratio of RE site to Ta ionic radius (r_A/r_B), bulk modulus (B), ionic bond strength (I_{A-B}), Clementi effective nuclear charge (Z-eff-C), melting point (MP), and temperature (T). Additionally, we plotted relationships between the features (excluding temperature) and thermal conductivity, as illustrated in Supplementary Fig. S3. The results indicate that none of the features exhibit a significant linear relationship with thermal conductivity, suggesting that thermal conductivity may be influenced by the combined effects of multiple features.

Among the eight regression algorithms evaluated, GBRT and XGBoost exhibited the highest cross-validation performance, with mean Coefficient of Determination (R^2) values of 0.950 and 0.949 and mean Root Mean Square Error (RMSE) values of 0.106 and 0.111 $\text{W m}^{-1} \text{K}^{-1}$, respectively (Supplementary Fig. S4). Based on these two models, we fixed the temperature and traversed all possible feature combinations of the remaining 9 features after the correlation analysis, training models for each combination while recording the R^2 and RMSE values for both models. The feature-subset analysis showed that the GBRT model overall outperforms XGBoost, and the model performance improved markedly when the number of descriptors increased from two to three but plateaued thereafter (Fig. 2b). The combination of T, Z-eff-C and I_{A-B} was therefore selected as the minimum predictive feature set. Using these features, the GBRT model achieved an R^2 of 0.832 on the test set (Fig. 2c), indicating lower generalization performance than suggested by cross-validation ($R^2 = 0.950$).

From a physical mechanism perspective, Z-eff-C (effective nuclear charge) determines the strength of interatomic interactions and the stiffness of chemical bond, thereby influencing lattice binding energy and phonon group velocity, which ultimately affects thermal conductivity.^[61, 62] Meanwhile, I_{A-B} (ionic bond strength) reflects the ionicity characteristics of chemical bonds and the asymmetry of local charge distribution. It is related to the electrostatic attraction between cations and anions and the bond polarization effects, which alter the bond lengths and angles of RE–O/Ta–O bonds and introduce local lattice distortions and lattice strain fields.^[63-65] This ionicity-driven microstructural heterogeneity modulates phonon scattering behavior, thereby exerting a significant influence on lattice thermal conductivity.

Model Pre-training and Transfer learning

Although the GBRT model achieved a prediction accuracy of $R^2 = 0.832$ on the independent test set, this still falls short of the high-precision requirements for practical applications of thermal conductivity prediction. The model's accuracy is constrained by

insufficient data volume and sample sparsity. The introduction of transfer learning technology offers an effective approach to addressing sparse small-sample problems. In addition to RETaO₄, this work systematically compiled thermal conductivity data for other thermal barrier coating systems, including rare-earth niobates, zirconates, and cerates, thereby establishing a multi-system dataset. (Details in Supplementary Table S3 and Fig. S5).^[50, 66-79]

For the multi-material system dataset, we constructed source-domain models with varying neural network parameters and evaluated their performance. The models with 3, 4, and 5 layers exhibited similar cross-validation performance, with R^2 values of 0.801, 0.823, and 0.802, and RMSE values of 0.247, 0.226, and 0.247, respectively (Supplementary Figs. S6a-c). After comprehensively evaluating model performance and generalization ability, we ultimately selected the 4-layer architecture as the optimal solution. Without target-domain fine-tuning, however, all source-domain models performed poorly on the RETaO₄ test set ($R^2 < 0.5$; $RMSE > 0.30 \text{ W m}^{-1} \text{ K}^{-1}$; Supplementary Figs. S6d-f), indicating that deep neural network models (DNN) trained solely on large multi-material systems cannot accurately capture the thermal conductivity variation patterns of RETaO₄ materials. Further adoption of transfer learning strategies is required.

The four-layer source model was subsequently fine-tuned on the RETaO₄ dataset by freezing its first one, two or three layers, denoted Progressive Fine-tuning (PFT), Balanced Fine-tuning (BFT) and Lightweight Fine-tuning (LFT), respectively (Fig. 2d).

The results of cross-validation and test set using three different fine-tuning strategies for the models can be seen in Fig. 2e and Supplementary Fig. S7. All three fine-tuning strategies demonstrably improved the R^2 on the independent test set. Among them, BFT achieved the highest R^2 (0.909), PFT reached $R^2 = 0.904$, and LFT yielded $R^2 = 0.896$. A four-layer network trained directly on RETaO₄ achieved cross-validation and test set R^2 values of 0.942 and 0.870, respectively (Supplementary Fig. S8).

Fig. 2g illustrates the performance of different modeling strategies on the independent RETaO₄ test set. All three fine-tuning strategies outperform both the GBRT model and the deep neural network trained solely on the small RETaO₄ dataset (details in Supplementary Table S4). This demonstrates the effectiveness of transfer learning in addressing the issue of insufficient generalization capability caused by limited data. BFT provided the highest test performance and was therefore used for subsequent composition screening.

To examine how the BFT model used the selected descriptors, global feature importance was quantified using the normalized mean absolute SHAP value. Temperature was the most influential input, followed by Z-eff-C and I_{A-B} (Fig. 2f). The substantial contributions of both composition descriptors show that the transfer model did not rely solely on the temperature dependence of thermal conductivity, but also incorporated variations in bond stiffness and local ionic interactions. Together, these results establish a compact and physically interpretable transfer-learning model for

predicting the thermal conductivity of compositionally complex RETaO_4 materials.

Virtual screening of multicomponent RETaO_4 compositions

We applied the BFT model to a virtual space containing 300,564 five- to eight-component RETaO_4 compositions generated from 12 rare-earth elements. We then calculate two key features for these compositions: $I_{\text{A-B}}$ and $Z\text{-eff-C}$. Fig. 3a illustrates the feature distributions of the composition space and various datasets. It is evident that the constructed composition space almost completely covers the original RETaO_4 dataset, significantly expanding the boundaries along both feature dimensions. This demonstrates the comprehensiveness and representativeness of the constructed composition space. Meanwhile, we compared the feature ranges of the multi-system dataset with those of the RETaO_4 dataset and composition space (see Supplementary Table S6). The multi-system dataset exhibits a substantially broader feature distribution range, far exceeding that of the single RETaO_4 system. This large span and wide coverage of the source domain are crucial for achieving effective transfer to the small-sample RETaO_4 target domain.

At $T = 900\text{ }^\circ\text{C}$, $I_{\text{A-B}}$ and $Z\text{-eff-C}$ were used as inputs to the GBRT and BFT models to predict the thermal conductivity of all candidate compositions. The construction of the composition space is described in Methods, with the number of candidates in each compositional category provided in Supplementary Table S5.

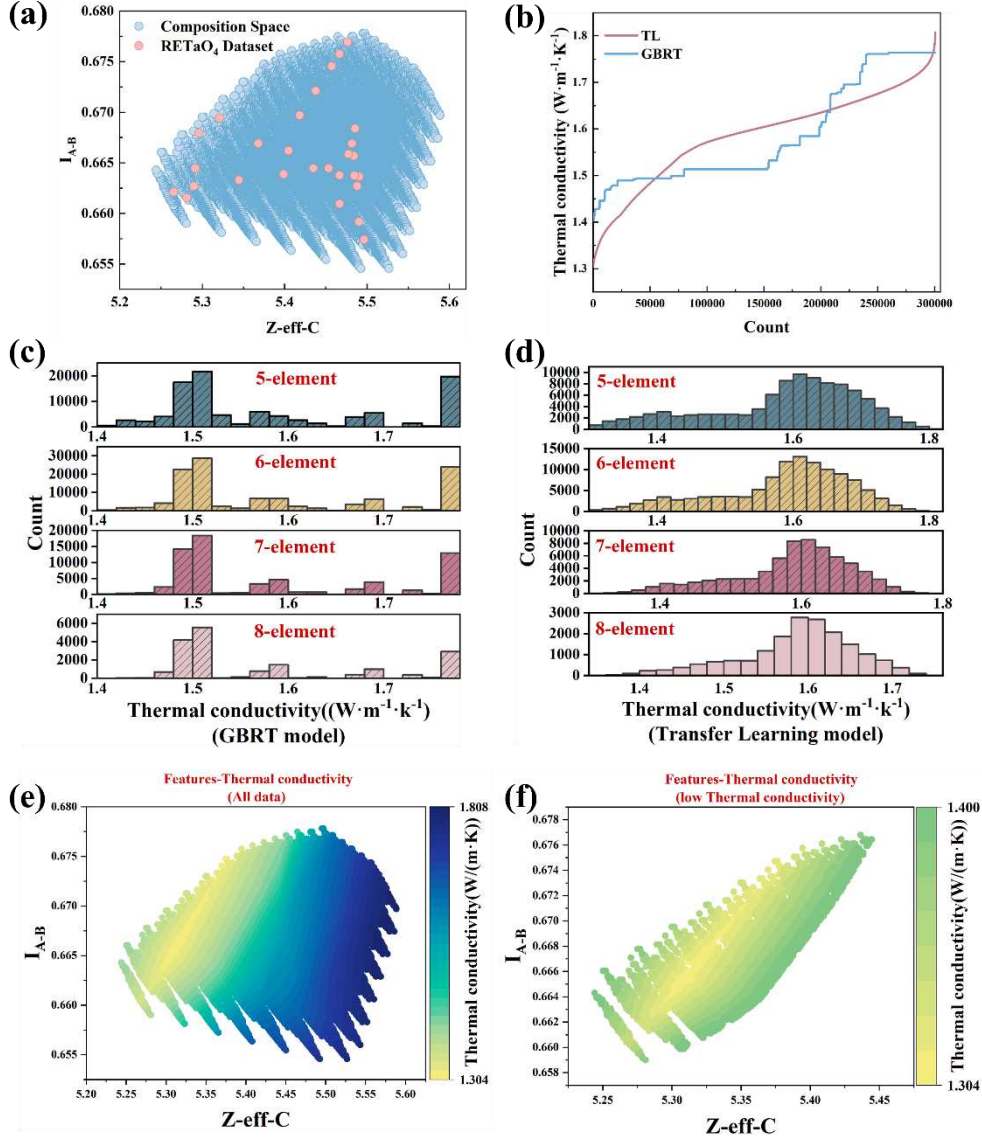


Figure 3. (a) Feature Distribution of the RETaO₄ Dataset and Composition Space. (b) Prediction distribution curves for thermal conductivity from the transfer learning model and GBRT model (c) Prediction distribution histogram of the GBRT model in the compositional space (d) Prediction distribution histogram of the transfer learning model in the compositional space. (e) Relationship between thermal conductivity and feature mapping across the entire compositional space (f) Relationship between thermal conductivity and feature mapping within the low thermal conductivity region

Fig. 3b compares the rank-ordered thermal-conductivity predictions of the GBRT and BFT models across the composition space. The GBRT predictions exhibit pronounced plateaus, whereas the BFT model produces a broader and more continuous distribution. The corresponding histograms (Figs. 3c-d) confirm that this difference persists across the 5–8-component spaces: GBRT predictions cluster at several discrete values, while the BFT model resolves gradual variations among compositions. This

behavior reflects the piecewise-constant output of tree-based regression and the greater ability of the neural-network model to distinguish subtle changes in continuous descriptors. Together with its higher performance on the test set ($R^2 = 0.909$, compared with 0.832 for GBRT), these results demonstrate that the BFT model provides superior generalization and compositional resolution for large-scale screening.

Fig. 3e displays the relationship between the predicted thermal conductivity and features across the entire composition space. It can be seen that the low thermal conductivity region is concentrated in a diagonal band-like, and thermal conductivity shows a clear upward trend with increasing Z-eff-C. This phenomenon suggests that the effective charge parameter Z-eff-C exerts a significant positive regulatory effect on thermal conductivity.

Further, we plotted the feature-thermal conductivity relationship curve for the low thermal conductivity region (thermal conductivity $< 1.4 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$), as shown in Fig. 3f, the low thermal conductivity phenomenon is concentrated in the central region. When Z-eff-C is fixed, increasing I_{A-B} leads to a decrease in thermal conductivity, which begins to rebound after reaching a certain threshold. This suggests that the optimal combination of these two features may be the key factor determining low thermal conductivity. Within the range where Z-eff-C $\approx 5.30 - 5.35$ and $I_{A-B} \approx 0.664 - 0.670$, thermal conductivity is generally low, constituting the ideal target region for material optimization.

Experimental Validation

To screen for components with low thermal conductivity, we select one representative composition from each of the 5-component, 6-component, 7-component, and 8-component spaces for experimental preparation and validation. During the composition selection process, priority is given to composition with low predicted thermal conductivity and high rankings, while also favoring elements with higher importance rankings. As the number of components increases, emphasis is placed on the systematic design of compositions and the ability to maintain continuity in elemental composition, ensuring that higher-component combinations gradually incorporate new elements based on lower-component compositions. Based on these selection criteria, the following representative compositions have been chosen for experimental preparation: $\text{Y}_{0.40}\text{Ce}_{0.10}\text{Sm}_{0.30}\text{Gd}_{0.10}\text{Er}_{0.10}\text{TaO}_4$ (5RE), $\text{Y}_{0.40}\text{Ce}_{0.10}\text{Sm}_{0.20}\text{Eu}_{0.10}\text{Gd}_{0.10}\text{Dy}_{0.10}\text{TaO}_4$ (6RE), $\text{Y}_{0.40}\text{Ce}_{0.10}\text{Sm}_{0.10}\text{Eu}_{0.10}\text{Gd}_{0.10}\text{Dy}_{0.10}\text{Yb}_{0.10}\text{TaO}_4$ (7RE), and $\text{Y}_{0.30}\text{Ce}_{0.10}\text{Sm}_{0.10}\text{Eu}_{0.10}\text{Gd}_{0.10}\text{Dy}_{0.10}\text{Ho}_{0.10}\text{Yb}_{0.10}\text{TaO}_4$ (8RE).

Rietveld refinement showed that the diffraction patterns of all four samples were well described by the monoclinic YTao_4 structure with space group $C2/c$, yielding goodness-of-fit values of 1.475–1.557. Their relative densities ranged from 97.57% to 99.87%, and SEM–EDS mapping showed spatially homogeneous distributions of the constituent elements. Full refinement patterns, elemental maps are provided in

Supplementary Figs. S9-S10, whereas the refined structural parameters and acoustic and mechanical properties are summarized in Supplementary Tables S7-S8. XPS analysis confirmed successful doping of rare earth ions in all samples (Supplementary Fig. S9e). Deconvolution of the O 1s spectra revealed three components—lattice oxygen, physically adsorbed oxygen, and oxygen vacancies—consistent with prior studies (Supplementary Fig. S9f), corroborating that oxygen vacancy defects in the lattice contribute to the reduction in thermal conductivity.^[80-83]

Next, we measured the thermal diffusivity of the four samples over a temperature range from room temperature to 900 °C and calculated their thermal conductivities. Figs. 4a–d illustrate the comparison between experimentally measured thermal conductivity and predictions from the transfer learning model for 5RE, 6RE, 7RE, and 8RE samples at different temperatures. At 900 °C, the experimental thermal conductivities for the 5RE, 6RE, 7RE, and 8RE samples are 1.276 W·m⁻¹·K⁻¹, 1.470 W·m⁻¹·K⁻¹, 1.341 W·m⁻¹·K⁻¹, and 1.307 W·m⁻¹·K⁻¹, respectively, while the predicted values of model are 1.304 W·m⁻¹·K⁻¹, 1.305 W·m⁻¹·K⁻¹, 1.306 W·m⁻¹·K⁻¹, and 1.359 W·m⁻¹·K⁻¹. The small discrepancies between experimental and predicted values indicate that the model exhibits relatively reliable predictive performance at elevated temperatures. It is worth noting that the thermal conductivities of the 5RE and 8RE samples at 900 °C are 1.276 W·m⁻¹·K⁻¹ and 1.307 W·m⁻¹·K⁻¹, respectively, both lower than the lowest thermal conductivity value (1.322 W·m⁻¹·K⁻¹) in the dataset at 900 °C. This result aligns closely with our research objective of screening for low-thermal-conductivity multicomponent thermal barrier coating materials. Although the thermal conductivities of the 6RE and 7RE samples did not fall below the lowest value in the dataset, their overall thermal insulation performance remains highly impressive.

Fig. 4e compares the thermal conductivities of the four samples in this work with the following materials: the thermal barrier coating materials with the lowest thermal conductivity for each corresponding number of components in the RETaO₄ dataset, the component with the lowest thermal conductivity in the RETaO₄ dataset. The equimolar materials we synthesized containing the same elements as the candidate materials. (respectively designated as 5RE_eq, 6RE_eq, 7RE_eq, and 8RE_eq; details can be found in Supplementary Table S9 and Fig. S11) and typical thermal barrier coating materials such as rare-earth niobates, zirconates, and cerates. The comparison results reveal that the four samples all exhibit excellent thermal conductivity performance, with the 5RE sample exhibiting the lowest thermal conductivity reported to date for bulk RETaO₄ at 900 °C (see Table S9 for details). It is worth noting that the thermal conductivities of the four non-equimolar compositions designed in this work are all lower than those of their corresponding equimolar counterparts. This indicates that the conventional high-entropy strategy of directly adopting equimolar mixing does not necessarily guarantee the lowest thermal conductivity; rather, on the basis of the same constituent elements, further optimizing the component proportions can yield an even lower thermal conductivity. This result differs from the trend expected from the traditional equimolar strategy and thus experimentally verifies the effectiveness of the

composition-design strategy employed in this work. Meanwhile, this work measured the thermal expansion coefficients of these four materials (specific temperature-thermal expansion curves are available in Supplementary Fig. S12) and conducted a comparative analysis with typical thermal barrier coating materials. As shown in Fig. 4f, while these materials exhibit excellent low thermal conductivity characteristics, they also maintain a relatively high thermal expansion coefficient, demonstrating favorable comprehensive thermophysical properties.

Local structural disorder and phonon localization

To identify the atomistic origin of the lower thermal conductivities of 5RE and 8RE, we examined their local structural and vibrational properties using first-principles calculations. The lattice-distortion distributions of 5RE and 8RE were broader than those of 6RE and 7RE, as reflected by their larger interquartile ranges and extended high-distortion tails (Fig. 5a). The nearest-neighbor RE–O force constants exhibited a similar trend: 5RE and 8RE showed broader distributions than 6RE and 7RE (Fig. 5b–e), indicating greater heterogeneity in local bond stiffness. Such structural and bonding heterogeneity can disrupt local lattice periodicity and enhance vibrational mismatch, thereby impeding phonon propagation.^[84]

The phonon participation ratio (PPR) further reveals the dynamic consequence of such local structural disorder.^[85, 86] As shown in Fig. 5f–g, both 5RE and 8RE exhibit a large number of localized vibrational modes with low participation ratios ($\text{PPR} < 0.3$) in the low-frequency (0–5 THz) and medium-frequency (4–16 THz) regions. A low participation ratio indicates that only a limited number of atoms participate in a given vibrational mode, implying pronounced phonon localization. Under these conditions, vibrational energy becomes spatially confined and cannot efficiently contribute to long-range heat transport, thereby reducing the lattice thermal conductivity.

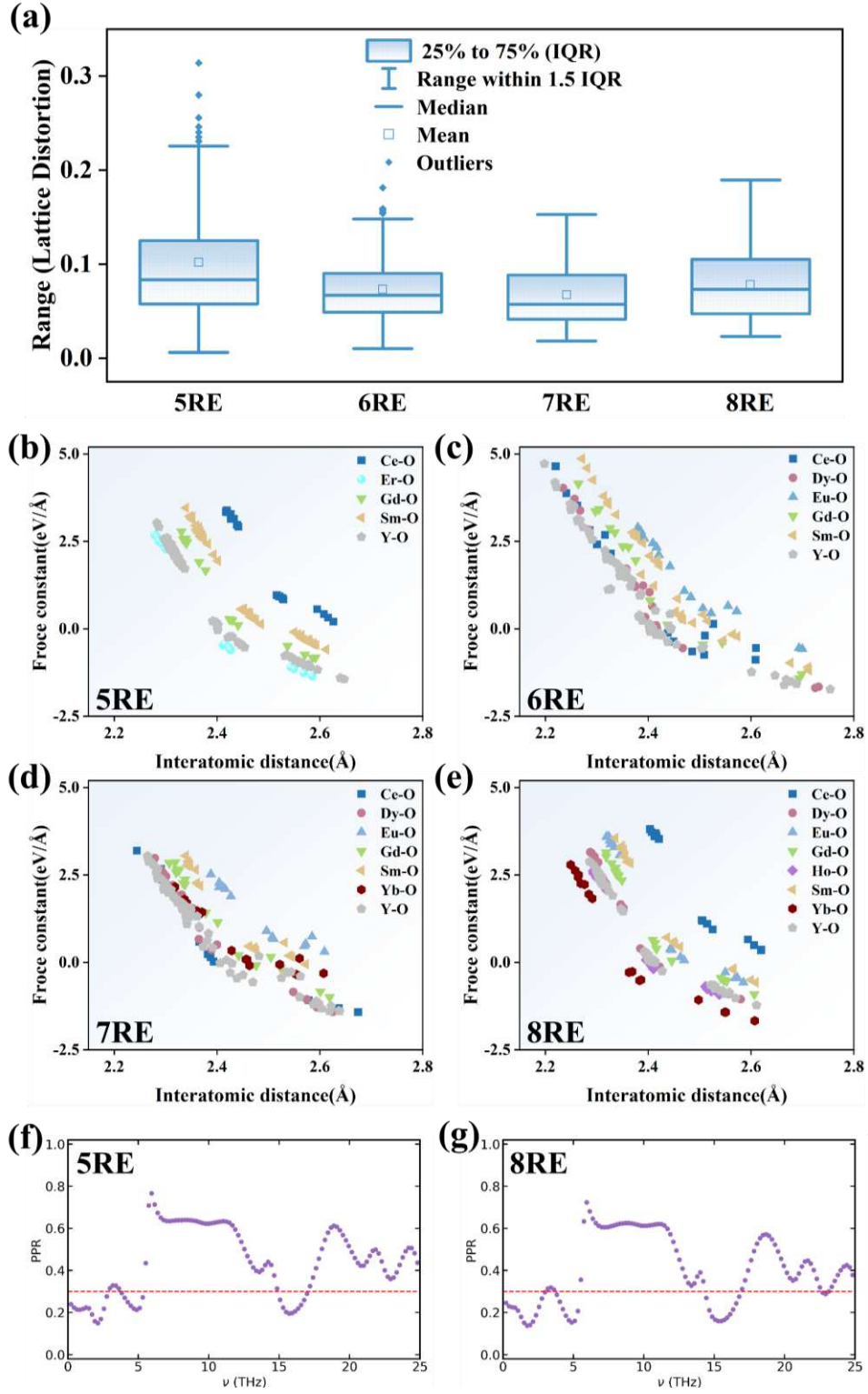


Figure 5. Calculation results of lattice distortion, force constants and PPR for RE samples. (a) Lattice distortion. Force constants of (b) 5RE; (c) 6RE; (d) 7RE; (e) 8RE. PPR of (f) 5RE; (g) 8RE

Multiscale phonon scattering in 5RE

TEM observations provide further direct microstructural evidence for the aforementioned mechanism. Fig. 6a presents atomic-resolution energy-dispersive X-ray (EDX) mapping, in which the distinct lattice positions of metal atoms demonstrate that the atomic arrangement within the multicomponent solid solution remains well-ordered. As shown in Fig. 6b, these parallel stripe-like structures with different orientations are identified as ferroelastic domains.^[9, 13, 72, 87] The ADF image in Fig. 6c shows that the interplanar spacings on both sides of the domain boundary are 2.663 and 2.753 Å, respectively, corresponding to approximately 3.3% interplanar mismatch. Such structural discontinuity at the domain boundary can effectively scatter low-frequency phonons. Meanwhile, the FFT patterns on both sides of the domain boundary indicate that the two variants correspond to the same crystal plane and can overlap after a rotation of about 3°, suggesting the presence of rotational twins with different orientations. Figs. 6e-f further reveal the presence of high-density dislocations in the sample. These dislocations can pin the ferroelastic domain walls, restrict their movement, and enhance the scattering associated with the domain walls. In addition, the FFT patterns at both ends of the dislocation region exhibit an orientation difference close to 90°, indicating the presence of strong local crystallographic distortion around the defect region. Therefore, ferroelastic domains and dislocations not only reflect the existence of local structural mismatch, but also provide additional scattering centers for low- and mid-frequency phonons.

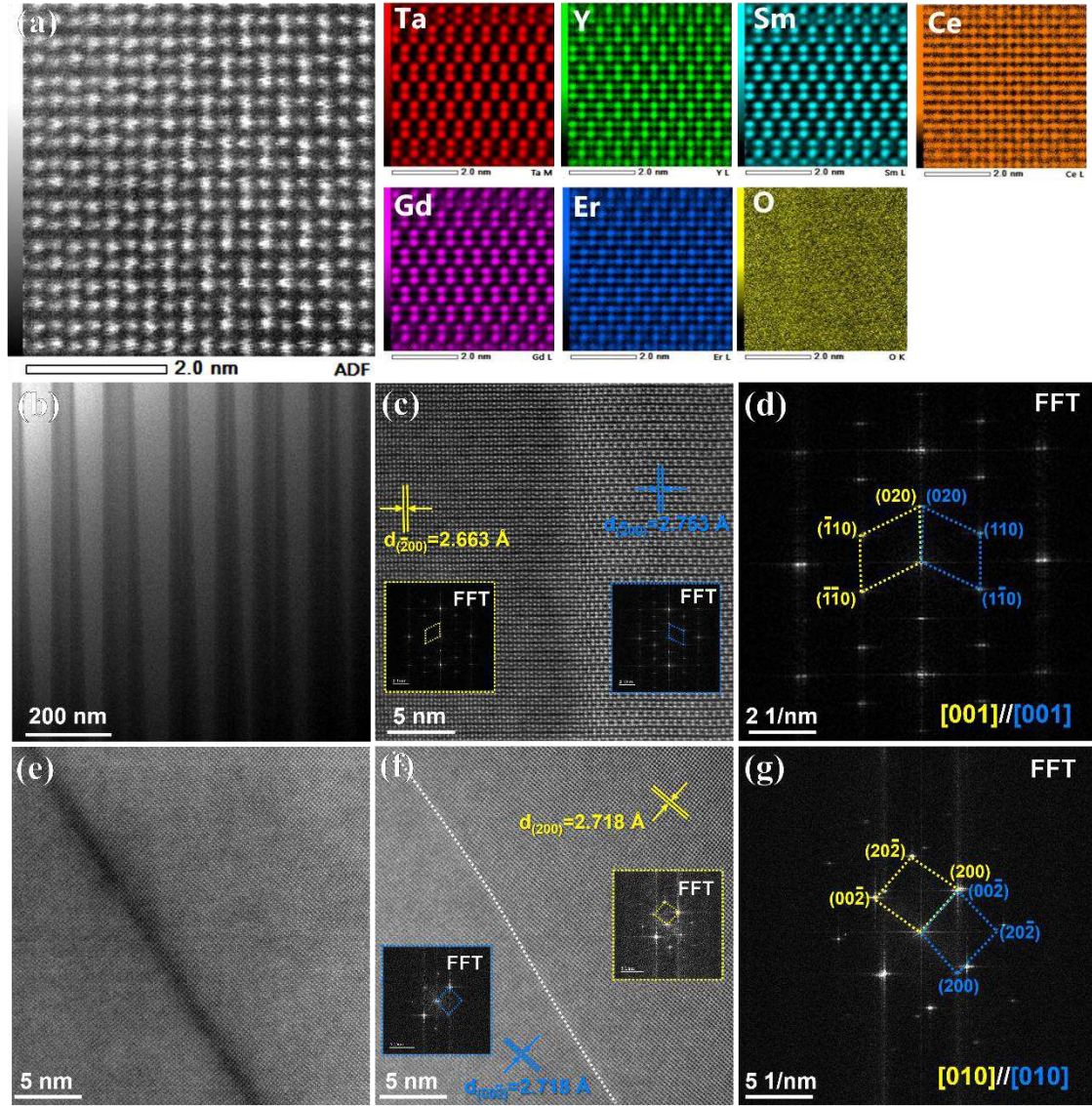


Figure 6. Microstructure and crystallographic characterization of ferroelastic domains in 5RE (a) EDX maps (b) Parallel strip morphology of ferroelastic domains (c) ADF image of the ferroelastic domain region (d) Fourier transform diffraction spots on both sides of the ferroelastic domain boundary (e) ABF image of the dislocation region (f) ADF image of the dislocation region (g) Fourier transform diffraction spots on both sides of the dislocations

To assess how defects spanning different length scales influence thermal transport in 5RE, its lattice thermal conductivity was analysed using a Debye–Callaway model incorporating Umklapp, grain-boundary, domain-boundary, point-defect and dislocation scattering (Methods).

Fig. 7a shows the phonon populations affected by different scattering at different frequencies for 5RE. The domain boundaries (DB) and grain boundaries (GB) mainly affect low-frequency phonon ($\tau_{DB}^{-1} \propto \omega^0$, $\tau_{GB}^{-1} \propto \omega^0$) scattering, and dislocation (D) affects mid-frequency phonon ($\tau_D^{-1} \propto \omega^1$) scattering. Umklapp scattering (U) and point

defect scattering (PD) mainly affect high frequency phonon ($\tau_U^{-1} \propto \omega^2, \tau_{PD}^{-1} \propto \omega^4$) scattering. Fig. 7b illustrates the impact of various scattering mechanisms on the spectral thermal conductivity. The results indicate that the lattice thermal conductivity is significantly suppressed across the entire frequency spectrum due to multiple scattering mechanisms.^[88, 89] Compared to the higher thermal conductivity observed when only intrinsic Umklapp scattering is considered, the introduction of GB and DB significantly reduces the thermal conductivity in the low-frequency region.^[21, 88] This reduction is attributed to the unique ferroelastic domain structure characteristic of rare-earth tantalates, where the domain size is 250–800 times the mean free path of phonon, enabling domain walls to effectively facilitate phonon scattering. Meanwhile, point defect (PD) scattering significantly inhibits thermal conductivity in the mid-to-high frequency range,^[21] specifically, the 5RE sample exhibits substantial lattice distortion (10%) and lattice spacing mismatch (3.3%), and XPS results further confirm the presence of internal oxygen vacancies, both of which work in concert to scatter mid-to-high frequency phonons. Furthermore, in conjunction with the dislocation lines observed in Fig. 6e, dislocation scattering (D) further enhances the suppression of mid-to-low frequency phonons, thereby achieving consistently low thermal conductivity across the entire frequency spectrum. Fig. 7c displays the lattice thermal conductivity fitted by the Debye-Callaway model at different temperatures, demonstrating that multidimensional lattice defects make a significant contribution to phonon scattering and the reduction in thermal conductivity. All calculation parameters can be found in Supplementary Table S10. In summary, as shown in Figs. 7d-g, the low thermal conductivity of 5RE ceramics is primarily attributed to phonon scattering within the lattice, induced by lattice distortion, oxygen vacancies, grain boundaries, ferroelastic domain structures, and dislocations.^[88, 90]

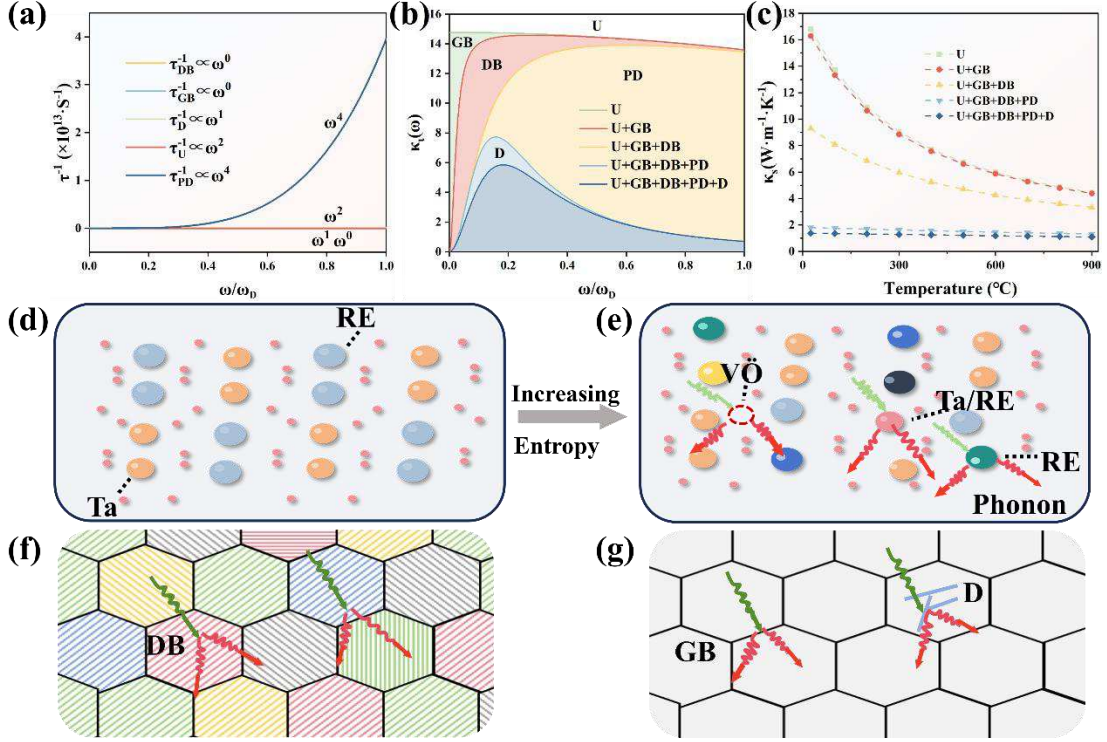


Figure 7. Thermal transport properties with different phonon scattering mechanisms in 5RE and Schematic illustration of phonon scattering mechanisms (a) Phonon relaxation times as a function of angular frequency at $T = 300 \text{ K}$; (b) Spectral lattice thermal conductivity at 300 K, including Umklapp scattering (U), grain boundary scattering (GB), domain boundary scattering (DB), point defect scattering (PD), dislocation scattering (D); (c) Fitted lattice thermal conductivity using the Debye-Callaway model. (d)-(e) Phonon scattering with severe lattice distortion and oxygen vacancies; (f) Phonon scattering targeting domain boundaries; (g) Phonon scattering targeting grain boundaries and dislocation.

Discussion

Cross-system transfer learning succeeded where direct prediction did not because chemically distinct thermal-barrier-coating oxides share common phonon-transport physics. Feature selection reduced the composition space to two minimal, physically interpretable descriptors beyond temperature: $Z\text{-eff-C}$ and $I_{\text{A-B}}$. $Z\text{-eff-C}$ reflects effective nuclear attraction and bond stiffness, thereby governs phonon group velocity, whereas $I_{\text{A-B}}$ captures bond ionicity and local charge heterogeneity, which promote local distortion and phonon scattering. The tree ensemble method of GBRT partitions descriptor space into discrete regions and assigns a nearly constant output within each terminal region. Consequently, small changes in continuous compositional descriptors may not alter the prediction until a tree threshold is crossed, producing the discrete prediction levels observed across the virtual composition space. By contrast, a neural network represents the property landscape through continuous nonlinear

transformations, but direct training on the small RETaO₄ dataset remains susceptible to insufficient sampling and overfitting. Transfer learning combines the advantages of both data scales: pretraining on the broader source-domain dataset allows the network to encode reusable relationships among temperature, effective nuclear charge, ionic bonding and thermal transport, whereas fine-tuning adjusts these representations to the specific distribution of RETaO₄. This explains why the BFT model outperformed both GBRT and the target-only neural network on the RETaO₄ dataset. The poorer performance of the source-only model confirms that source-domain knowledge is useful only after target-specific adaptation. Importantly, the evidence for the superiority of the transfer model is provided by its test set performance and experimental validation, rather than merely by the smoother distribution of its predictions.

The lower conductivity of the 5RE composition relative to the 6RE, 7RE and 8RE compositions is instructive: increasing the number of constituent elements does not monotonically reduce thermal conductivity. Instead, the identities and fractions of the constituent cations must generate the appropriate combination of bonding contrast, local distortion and defect structure. The experimentally validated compositions therefore illustrate the advantage of descriptor-guided non-equimolar design over empirical strategies based solely on the number of components.

Characterization and modelling indicate that the ultralow thermal conductivity arises from a hierarchy of mutually reinforcing mechanisms rather than a single defect class. At the atomic scale, broad distributions of lattice distortion and RE–O force constants, together with point defects such as oxygen vacancies and compositional mass and strain fluctuations, disrupt periodicity, localize vibrational modes and strengthen scattering in the middle- and high-frequency ranges. At the nanometre scale, TEM of the 5RE sample reveals ferroelastic domain boundaries and dense dislocations, dislocation pinning also stabilizes a dense domain-wall network, which extends scattering to scattering across low- and intermediate-frequency modes. At the micrometre scale, grain boundaries limit long-wavelength phonons. The Debye–Callaway analysis connects these observations to their spectral consequences. Together, DFT-derived phonon localization, TEM-observed domain and dislocation structures and transport modelling describe different levels of a single multiscale suppression mechanism rather than independent explanations.

Two caveats qualify this interpretation. First, the transfer benefit depends on shared phonon physics and diminishes for target oxides whose physics diverges from the source set. Second, the long-term thermal-cycling stability of these multi-component phases remains to be established. In summary, we have established a cross-system transfer learning framework for discovering low-thermal-conductivity RETaO₄ materials from limited target-domain data. This strategy is not only applicable to rare-earth tantalate systems but also reveals a general pathway for integrating multi-system material data and exploiting cross-system physical commonalities to achieve efficient material design. This work demonstrates that the paradigm of combining physical understanding with transfer learning holds promise as an efficient solution to the

challenge of small-sample material discovery.

Methods

Machine learning

Pearson Correlation Analysis: Pearson correlation analysis is a statistical method used to measure the strength and direction of the linear relationship between two continuous variables. Its core principle involves calculating the ratio of the covariance between the two variables to the product of their standard deviations, thereby yielding a correlation coefficient ranging from -1 to 1. The formula is as follows:

$$r = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2} \cdot \sqrt{\sum_{i=1}^n (y_i - \bar{y})^2}} \quad (1)$$

Where x_i and y_i represent the i -th observed values of the two variables, $\bar{x}$ and $\bar{y}$ denote the means of the two variables, and n is the sample size. When $r = 1$, it indicates a perfect positive linear correlation, meaning one variable increase linearly as the other increases. When $r = -1$, it indicates a perfect negative linear correlation, meaning one variable decrease linearly as the other increases. When $r = 0$, it indicates no linear correlation, meaning there is no linear relationship between the two variables.

Root Mean Square Error: The root mean square error (RMSE) is the square root of the mean square error. It retains the property of amplifying errors while ensuring that the error units are consistent with the original data, making it more interpretable. The formula is:

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (2)$$

where n is the sample size, y_i is the true value, $\hat{y}_i$ is the predicted value.

Coefficient of Determination: The R^2 score indicates the degree to which a model fits the data, with values ranging from $(-\infty, 1]$. The formula is:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (3)$$

where n is the sample size, y_i is the true value, $\hat{y}_i$ is the predicted value, $\bar{y}$ is the mean of the true values. When $R^2 = 1$, the model perfectly fits the data; when $R^2 = 0$, the model's predictive performance is equivalent to using the mean of the data; if R^2 is negative, the model's predictions are worse than simply using the mean.

Transfer Learning: The core idea of transfer learning is to apply knowledge learned from one domain or task to another related yet distinct domain or task, thereby enhancing the performance of the target task. Unlike traditional machine learning methods, transfer learning leverages knowledge from the source task (typically possessing vast amounts of data) to improve learning outcomes on the target task (often constrained by limited data), making it particularly suitable for scenarios with small datasets or high data acquisition costs.

Shared Model Parameters for Source and Target Tasks:

$$\theta_{\text{target}} = \theta_{\text{shared}} \cup \theta_{\text{target-specific}} \quad (4)$$

Where, θ_{target} is the target task, represents the parameters shared between the source and target tasks, and $\theta_{\text{target-specific}}$ denotes the parameters specific to the target task.

Model screening and feature selection

Eight regression algorithms were optimized by grid search and evaluated using 10 repetitions of 10-fold cross-validation. R^2 and RMSE were used as the evaluation metrics. Following correlation-based descriptor reduction, temperature was retained in every candidate feature subset, and all combinations of the remaining descriptors were evaluated using GBRT and XGBoost. The smallest subset that maintained performance comparable to the best-performing model was selected for subsequent analysis. The final GBRT model was trained using 80% of the dataset and evaluated on the remaining 20%. SHAP values were calculated to quantify the contribution of each descriptor to the model predictions.

Virtual composition-space construction

Twelve rare-earth elements (Y, Ce, Nd, Sm, Eu, Gd, Dy, Ho, Er, Tm, Yb and Lu) were considered for the RE site. For each component number $n \in 5, 6, 7, 8$, unordered elemental subsets were selected from the 12 elements. The fraction of each selected element was constrained to a positive multiple of 0.1, with the total RE-site occupancy satisfying $\sum_{i=1}^n x_i = 1$

For a given n-element subset, the number of allowable fraction vectors was $\binom{9}{n-1}$. The total number of candidates was therefore:

$$\sum_{n=5}^8 \binom{12}{n} \binom{9}{n-1} = 300,564$$

I_{A-B} and Z-eff-C were calculated for each candidate using the same compositional

averaging rules applied to the training data. These descriptors, together with a fixed temperature of 900 °C, were used as inputs to the GBRT and transfer-learning models.

Theoretical calculation

First-principles calculations were carried out by the Vienna *Ab initio* Simulation Package (VASP) software based on density functional theory (DFT).^[91] The projector augmented wave (PAW) method was used to describe the interaction between electrons and ions,^[92] and the generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation function was used to describe the electron exchange correlation potential.^[93] In all calculations, the plane wave cutoff energy was set to 500 eV, where k mesh with a separation of 0.03 Å⁻¹ according to the Monkhorst–Pack method was adopted in the first Brillouin zone.^[94] The convergence criterion of structural optimization was that the stress of each atom was less than 0.01 eV/atom. The convergence criterion for electronic optimizations was 1×10^{-6} eV per atom for total energy, and the forces per atom were reduced to 5×10^{-3} eV/Å. Lattice-dynamics calculations were obtained by the Phonopy package,^[95] and the stretching force constant was calculated within the framework of density functional perturbation theory (DFPT) via linear-response approach.^[96]

Debye–Callaway modelling

The multiphonon scattering mechanisms in 5RE ceramics are conducive to reducing the lattice thermal conductivity (κ_l). While Umklapp scattering plays a dominant role in thermal resistance, it is also significantly influenced by dislocations, point defects, domain boundaries, and grain boundaries. To investigate the impact of these multiple scattering mechanisms on κ_l , calculations were performed using the classical Debye–Callaway model according to the following equations:^[97]

$$\kappa_l = \frac{k_B}{2\pi^2 v_m} \left(\frac{k_B T}{h} \right)^3 \int_0^{\theta_D/T} \tau_{tot}(x) \frac{x^4 e^x}{(e^x - 1)^2} dx \quad (5)$$

where $x = \hbar\omega/k_B T$ is the reduced phonon frequency; $\hbar$ and ω correspond to the reduced Planck constant and phonon angular frequency, respectively, k_B is the Boltzmann constant, and T is the absolute temperature. The total phonon relaxation time (τ_{tot}) is calculated using the following formula:^[65, 98]

$$\tau_{tot}^{-1} = \tau_U^{-1} + \tau_{GB}^{-1} + \tau_{DB}^{-1} + \tau_{PD}^{-1} + \tau_D^{-1} \quad (6)$$

where τ_U^{-1} , τ_{GB}^{-1} , τ_{DB}^{-1} , τ_{PD}^{-1} , and τ_D^{-1} represent the scattering rates of the Umklapp process, grain boundary scattering, domain boundary scattering, point defect scattering,

and dislocation scattering, respectively. The relaxation time (τ) for each mechanism is calculated according to the following formulas:^[66, 99-103]

$$\tau_U^{-1} = \frac{2}{(6\pi^2)^{1/3}} \frac{k_B \bar{V}^{1/3} \gamma^2 \omega^2 T}{\bar{M} v_m^3} \quad (7)$$

$$\tau_{GB}^{-1} = \frac{v_m}{d_{GB}} \quad (8)$$

$$\tau_{DB}^{-1} = A \frac{v_m}{d_{DB}} \quad (9)$$

$$\tau_{PD}^{-1} = \frac{\bar{V} \omega^4}{4\pi v_m^3} f_i \left[\varepsilon \left(\frac{r_{i,s} - r_s}{r_s} \right)^2 + \left(\frac{M_{i,s} - \bar{M}_s}{\bar{M}_s} \right)^2 \right] \quad (10)$$

$$\tau_D^{-1} = 0.6 \times B_D^2 N_D \gamma^2 \omega \left[\frac{1}{2} + \frac{1}{24} \left(\frac{1-2\xi}{1-\xi} \right)^2 \left(1 + \sqrt{2} \left(\frac{v_l}{v_t} \right)^2 \right) \right] + N_D \frac{\bar{V}^{4/3} \omega^3}{v_m^2} \quad (11)$$

Where $\bar{V}$ and $\bar{M}$ correspond to the average atomic volume and average atomic mass, γ is the Grüneisen parameter, v_m is the average sound velocity, and ω is the phonon frequency; d_{GB} and d_{DB} correspond to the grain size and domain boundary width, respectively, while A is the domain boundary fitting parameter; f_i denotes the lattice defect concentration, $r_{i,s}$ and r_s represent the i -th species ionic radius and the mean ionic radius at atomic position s , $M_{i,s}$ and $\bar{M}_s$ correspond to the i -th species mass and the mean mass at position s ; N_D denotes the dislocation density, B_D is the magnitude of the Burgers vector, ξ is the Poisson's ratio, and v_l and v_t are the longitudinal and transverse sound velocities, respectively.

Experimental

The preparation of rare-earth tantalate samples employed a solid-state reaction method, with raw materials supplied by Aladdin China Co., Ltd. The specific experimental procedure is as follows: First, the raw material powders were dried at 1000 °C for 3 hours to remove organic impurities and adsorbed moisture. Subsequently, components were precisely weighed according to the predetermined stoichiometric ratios and placed into a clean ball-milling jar. The ball-milling process used agate beads as the grinding medium, with anhydrous ethanol (occupying 3/4 of the jar's volume) added as the milling medium. The mass ratio of large, medium, and small agate beads

was 2:1:1. The milling was performed using a QM-3SP2 planetary ball mill from Nanjing Instrument Factory at a speed of 350 rpm for 24 hours. After milling, the ball-milling jar was dried in a 70 °C oven for 24 hours to obtain uniformly mixed dry powder. The powder was then sieved through 200/400 mesh screens to achieve a uniform particle size distribution. Next, 1.5 g of the sieved powder was placed into a 15 mm diameter mold and pressed at 8 MPa for 2 minutes to form a 2 mm thick disc-shaped sample. Finally, the pressed sample was sintered in a muffle furnace at 1650 °C for 6 hours, then cooled to room temperature with the furnace to obtain a dense rare-earth tantalate bulk sample.

Property measurements

The thermal diffusivity (α) of the samples was measured across the room temperature–900 °C range utilizing a laser flash apparatus (Netzsch LFA 427, Bavaria, Germany). The thermal conductivity (κ') was subsequently calculated using the following equation:^[51]

$$\kappa' = \rho C_p \alpha \quad (12)$$

The density ρ was determined using the Archimedes principle, while the specific heat capacity C_p was estimated based on the Neumann–Kopp rule. Subsequently, the actual thermal conductivity (κ) was evaluated via Equation (13) to compensate for the effect of residual porosity:^[104]

$$\frac{\kappa'}{\kappa} = 1 - \frac{4}{3}\varphi \quad (13)$$

where φ is the porosity. Furthermore, thermal expansion properties were characterized using a thermomechanical analyzer (Netzsch TMA-402 F3, Germany). Concurrently, acoustic velocities were measured via the Advanced Ultrasonic Modulus Measurement System (UMS-100; TECLAB, Chelles, France). Based on these velocity measurements, the mean sound velocity (v_m), Poisson's ratio (ξ), Young's modulus (E), shear modulus (G), bulk modulus (B), Grüneisen parameter (γ), and Debye temperature (θ_D) were subsequently calculated as follows:^[105]

$$v_m = \left[\frac{1}{3} \left(\frac{1}{v_l^3} + \frac{2}{v_t^3} \right) \right]^{-\frac{1}{3}} \quad (14)$$

$$\xi = \frac{1-2(v_t/v_l)^2}{2-2(v_t/v_l)^2} \quad (15)$$

$$E = \frac{\rho v_l^2 (3v_l^2 - 4v_t^2)}{v_l^2 - v_t^2} \quad (16)$$

$$G = \frac{E}{2(1+\xi)} \quad (17)$$

$$B = \rho \left(v_l^2 - \frac{4}{3} v_t^2 \right) \quad (18)$$

$$\gamma = \frac{3}{2} \left(\frac{1+\sigma}{2-3\sigma} \right) \quad (19)$$

$$\theta_D = \frac{h}{k_B} \left(\frac{3N}{4\pi V} \right)^{\frac{1}{3}} \times v_m \quad (20)$$

where v_t and v_l denote the transverse and longitudinal sound wave velocities, respectively. The constants h and k_B correspond to Planck's constant and the Boltzmann constant, respectively. N is the number of atoms per unit cell, and V represents the unit-cell volume.

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Author Contributions

Conceptualization: X.C., J.H., Y.W.; **Methodology:** Y.W., J.H., S.-L.S., Z.-K.L., Z.L.; **Software:** Y.W.; **Data curation:** Y.W.; **Formal analysis:** Y.W., Y.L.; **Investigation:** Y.W., Y.L., F.T.; **Visualization:** Y.W., Y.L., F.T.; **Supervision:** X.C., J.H., S.-L.S., Z.-K.L., Y.J., J.F.; **Validation:** Y.W., J.H., Y.L., F.T.; **Writing – original draft:** Y.W.; **Writing – review & editing:** All authors; **Resources:** X.C., J.H., Y.J., J.F.; **Funding acquisition:** X.C., J.H.; **Project administration:** X.C., J.H.

Conflict of Interest

The authors declare no conflicts of interest.

Data Availability

Relevant data supporting the key findings of this study are available within the paper and the supplementary information file. Source data are provided with this paper. Source data are provided with this paper

Code Availability

The code and trained models are openly available at

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