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Accelerating Ceramic Materials Development via Machine Learning: A Critical Review

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Abstract

Ceramics are inorganic, non-metallic materials renowned for their exceptional thermal, mechanical, chemical, and functional properties, making them indispensable across aerospace, biomedical, electronic, and energy applications. Despite their advantages, optimizing ceramic processing remains a major challenge due to the complex interplay of temperature, particle characteristics, atmosphere, and additives, where minor deviations can significantly affect microstructure and performance. Traditional experimental and computational approaches are often time-consuming or resource intensive. Machine learning (ML) offers a transformative alternative by enabling accurate property prediction, process optimization, materials discovery, and degradation analysis. This review presents a comprehensive overview of ML applications in ceramics, literature examples, and discusses current challenges and future directions, highlighting the potential of ML to accelerate the design and development of high-performance ceramic materials.

Keywords: *Ceramic Materials, ML.*

I. INTRODUCTION

Ceramics are inorganic, non-metallic materials composed of metallic and non-metallic elements bonded predominantly through ionic and covalent interactions. They are typically produced by shaping fine powders into a "green body" and consolidating it through sintering, where particles bond and densify at high temperatures without fully melting. What makes ceramics particularly valuable is their unique properties: they can withstand extreme heat, resist wear and corrosion, and in many cases exhibit electrical, magnetic, or optical functionalities that metals and polymers cannot provide. These properties make ceramics indispensable in diverse sectors, ranging from aerospace turbines and biomedical implants to electronic devices, renewable energy technologies. In short, ceramics hold a vital place in both advanced engineering materials they combine strength, stability, and multifunctionality in ways few other materials can.

Yet, despite their promise, the manufacturing of ceramics—particularly optimizing sintering conditions—remains one of the field's greatest challenges. Sintering is a delicate balancing process: the ceramic remains porous and weak at too low a temperature; at too high a temperature, abnormal grain growth, warping, or even phase decomposition can occur. Beyond temperature, factors such as heating rate, particle size, distribution, impurities, and the surrounding atmosphere (air, inert, or reducing) strongly influence densification and defect formation. The use of dopants or sintering aids introduces further complexity, since their effects are highly sensitive to composition and concentration. Because of this intricate interplay of variables, even small deviations can lead to large differences in the final density, microstructure, and performance of ceramics. This complexity makes ceramic processing both scientifically fascinating and industrially demanding, creating a pressing need for more predictive, data-driven approaches.

Traditional methods of determining ceramic properties rely either on experimental trial-and-error processes, which are often costly and time-consuming, or on computational simulations, which require significant resources and large datasets [1]. Here, ML offers a transformative pathway. By identifying hidden patterns in complex datasets and predicting properties with remarkable accuracy, ML enables cost-effective design and optimization of ce-

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ramics. It can predict synthesizability, guide the exploration of vast compositional spaces, and accelerate the development of materials with tailored mechanical, thermal, or functional properties [2]. This integration of ML into ceramic research is not merely a technological upgrade—it represents a paradigm shift toward intelligent, data-driven materials science.

One of the most compelling advantages of ML in ceramics is its ability to predict properties from composition and processing parameters without exhaustive experimentation. For instance, [3] applied ML to predict the dimensions of laser-engraved channels in alumina ceramics, identifying optimal process parameters and enhancing product quality. Similarly, in manufacturing, ML enables more precise control of conditions such as temperature and pressure during sintering or machining, thereby improving reproducibility and reducing variability. In additive manufacturing, the optimization of process parameters such as printing speed, extrusion rate, and toolpath strategies has significantly influenced the mechanical performance and structural integrity of printed parts [4-6], and ML provides a powerful framework to accelerate this optimization. These predictive capabilities have profound implications for industries where ceramics play critical roles, from high-performance aerospace systems to everyday construction materials.

Beyond optimization, ML is also a powerful tool for materials discovery. For example, [7] combined finite element analysis with ML to simulate and optimize architectured interlocking ceramics, enabling accurate prediction of their performance under stress. Such approaches allow researchers to explore vast design spaces that would be impractical through trial-and-error methods alone, opening the door to advanced ceramics with specialized and unprecedented capabilities.

Another promising direction lies in understanding degradation and failure mechanisms, which are vital in applications requiring long-term reliability, such as biomedical implants or structural components of aircraft. By training on experimental datasets, ML models can predict how ceramics fail under certain conditions, enabling proactive improvements in design and processing to extend material lifespan [8]. These insights bridge the gap between laboratory performance and real-world durability, addressing one of the most pressing challenges in ceramic applications.

In summary, the integration of ML into ceramic research marks a new era of materials innovation. ML empowers researchers and manufacturers to move beyond empirical trial-and-error toward predictive, adaptive, and scalable strategies. Its ability to forecast properties, optimize processes, accelerate discovery, and model degradation mechanisms positions ML as a transformative tool in ceramics. By harnessing these capabilities, the field is poised for breakthroughs that can drive advances across industries while deepening our scientific understanding of this essential class of materials.

In this work, we present a comprehensive review of the applications of ML in the field of ceramic materials. The review begins with an overview of the different types of ML and a general workflow for predicting ceramic properties using ML models, followed by a summary of ML approaches applied to ceramics in the literature. It concludes by highlighting the major challenges associated with current ML methodologies and offering perspectives on future research directions for advancing ML-driven ceramic development.

II. ML IN CERAMIC MATERIALS

ML techniques can be broadly classified into four main types, each offering distinct opportunities for ceramic materials research. Supervised learning is the most widely applied, where models are trained on labeled datasets to predict properties such as hardness, dielectric constant, or fracture toughness from composition and processing parameters. Unsupervised learning plays an important role in exploring large, unlabeled datasets, for example clustering ceramic compositions with similar behavior or reducing the dimensionality of complex microstructural data. Semi-supervised learning bridges the gap when only limited experimental data are available, leveraging small & labeled datasets alongside larger unlabeled ones to improve property prediction and microstructure classification. Finally, reinforcement learning (RL) emerges as a powerful tool for process optimization, enabling the design of adaptive sintering schedules or autonomous experimental workflows. Together, these approaches expand the predictive and exploratory capabilities of ceramic research, accelerating discovery and optimization.

➢ *Supervised ML in Ceramic Materials*

Supervised ML training begins with data collection from literature or simulations/experiments, followed by data cleaning to remove samples with problematic features or labels. There are two approaches for data treatment- direct coding with numeric or feature engineering and data pre-treatments to guide ML models. Afterward, different ML models are trained and assessed with diverse parameters, and the top-performing model is chosen for making predictions. Predicted ceramics undergo filtering, with selected predictions synthesized and experimentally characterized for validation. Synthesized samples are then integrated into the database to enhance ML performance. Each step is tailored to ceramics, addressing challenges like missing data and ensuring accurate predictions, thereby advancing the rational discovery of high-performance ceramics [9].

- *Database construction*

ML in materials science relies heavily on high-quality databases, which have historically been limited in size. However, existing databases primarily feature ordered or simple structures, lacking chemically disordered ceramics. Consequently, ML applications for ceramics are hindered by the small dataset available. Although there are early attempts to build ceramics

databases, there are still difficulties, such as the varied structures of ceramics like perovskites and fluorites, which make ML predictions more complex. Moreover, most current ML models focus on specific types of ceramics, further limiting their applicability. Another challenge is the shortage of multi-phase samples in databases, as researchers often disregard materials with mixed phases as negative results. Nonetheless, efforts to compile ceramics databases are underway, with reviews documenting hundreds of published ceramics. Addressing these challenges is crucial for expanding the scope and effectiveness of ML in predicting and discovering ceramics with diverse compositions and properties [9] as shown in Fig. 1.

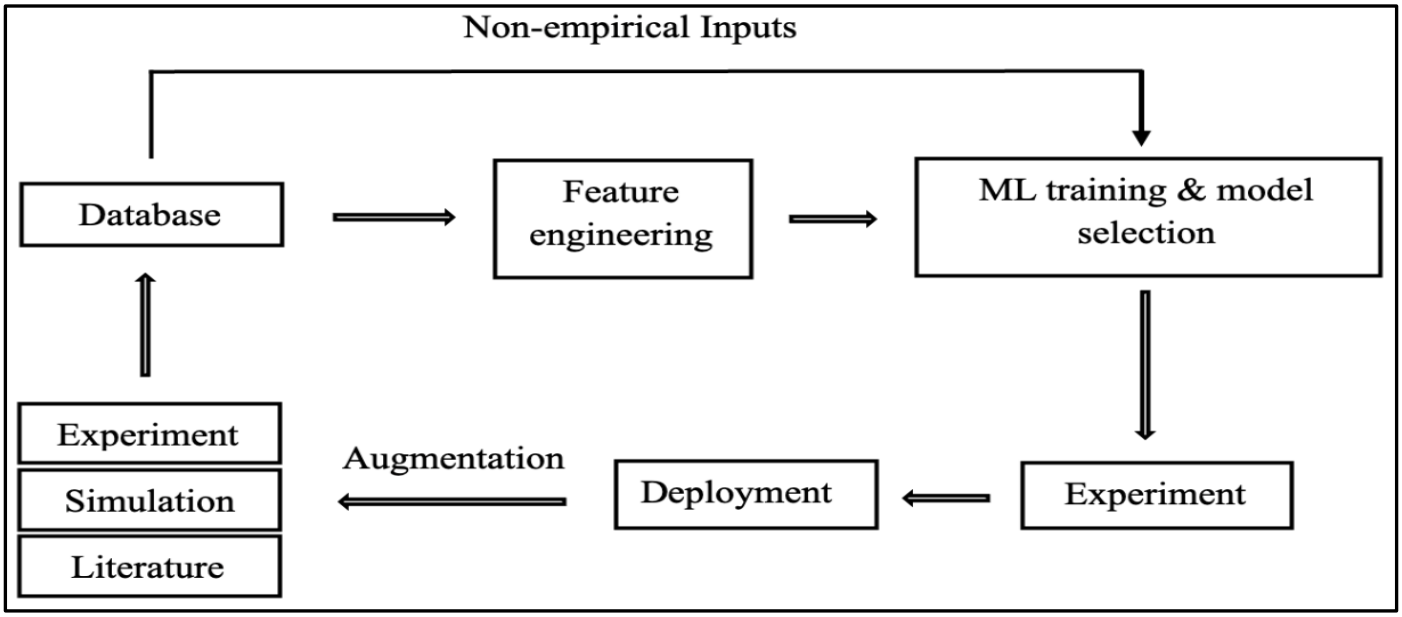

Fig 1 ML Workflow for Ceramic Materials.

- *Feature Engineering*

Before feeding ceramic compositions into ML models, the compositional details need to be converted into continuous or discrete variables so that the input features can be effectively matched with output labels. Three categories of input features exist. Initially, experience-independent features encode compositions numerically, usually using one coding for categorical variables. Each sample's size matches the number of elements, with a binary vector showing the presence of each element.

Multiplying these vectors by elemental concentrations shows the composition, but this representation lacks chemical insights, requiring large amounts of data and complex models for effective training. Secondly, atomic/precursory-based descriptors, like atomic radius and electronegativity, are directly obtained from the periodic table, requiring no additional calculations. These features are commonly employed in ML models for ceramic design. Thirdly, costlier experimental or simulation-based features, such as melting temperature and mixing enthalpy, provide valuable but expensive information.

While unsuitable as inputs due to cost, some are used as labels, offering detailed insights into target ceramics. For example, energy above the hull and entropy forming ability (EFA) were utilized as labels, with ML methods predicting EFA values, aiding in identifying multi-phase materials [9].

Overall, while experience-independent features demand extensive data and complex models, atomic/precursory-based descriptors offer straightforward input. Expensive experimental or simulated features, though valuable, are typically reserved for labeling due to their cost. This categorization facilitates efficient parameterization of compositions for ML-based design and prediction tasks.

Now, how ML-based ceramic is modeled is discussed here. At this stage, the formula of different parameters is discussed. The calculation of the atomic radius difference is derived as follows:

$$\delta = \sqrt{\sum_{i=1}^{n} c_i \left(1 - \frac{r_i}{\overline{r}}\right)^2} \qquad (1)$$

The concentration of the i-th precursor is denoted as c_i, its atomic radius as r_i, and the average atomic radius as $\overline{r} = \sum_{i=1}^{n} c_i r_i$. For many ceramic carbides, local lattice distortion impacts miscibility by reducing mixing enthalpy, influencing defect formation energies and mechanical properties through charge redistribution. Similarly, other atomic/precursory properties (valence electron concentration, electronegativity, volume, mass, density, and atomic radius) can be transformed into averages and deviations. The average properties are computed as:

$$\overline{p} = \sum_{i=1}^{n} c_i p_i \qquad (2)$$

In this context, p refers to precursory properties. These mean values provide a comprehensive overview of ceramic properties, adopting a mean-field approach. Moreover, the deviations serve to measure disparities among precursors, and they are determined through the following calculation:

$$\delta_p = \sqrt{\sum_{i=1}^{n} c_i \left(1 - \frac{p_i}{\overline{p}}\right)^2} \qquad (3)$$

The electronegativity difference (ΔX) is slightly different from equation (3):

$$\Delta X = \sqrt{\sum_{i=1}^{n} c_i \left(X_i - \overline{X}\right)^2} \qquad (4)$$

The mixing entropy is usually calculated by:

$$\Delta S = -R \sum_{i=1}^{n} c_i \ln c_i \qquad (5)$$

Here, R represents the gas constant. Maximizing ΔS occurs when there is an equal atomic ratio. Furthermore, changes in properties resulting from mixing (e.g., ΔH and ΔV) are determined through the following calculation:

$$\Delta p = p_{HEC} - \overline{p} \qquad (6)$$

Here, p_{HEC} denotes the property value of ceramic post-mixing. These alterations can measure the distinctions between ceramics and their precursors [9].

- *Model Selection and Interpretation*

In supervised ML, the dataset undergoes random division into training, validation, and test sets. The training set is utilized to teach the ML model, enabling it to discern the relationship between input and output by minimizing the variance between predicted and actual labels. The validation set is employed to compute metrics for hyperparameter adjustment. The test set comprises samples unseen during training, serving to gauge the generalization performance of the well-trained model. However, for smaller datasets, like newly developed ceramics, splitting into training and validation sets may result in bias due to uneven distribution of high-quality samples. To mitigate this bias, cross-validation (CV) is employed. In CV, the dataset is divided into n subsets, or n-fold CV, where each subset is treated as the validation set in turn, while the rest serve as training data. Model performance is then evaluated by averaging metrics across all models. The 5-fold and 10-fold CV methods are commonly used, balancing training burden and accuracy. This approach is frequently employed in literature for predicting the single-phase synthesizability of ceramics [9].

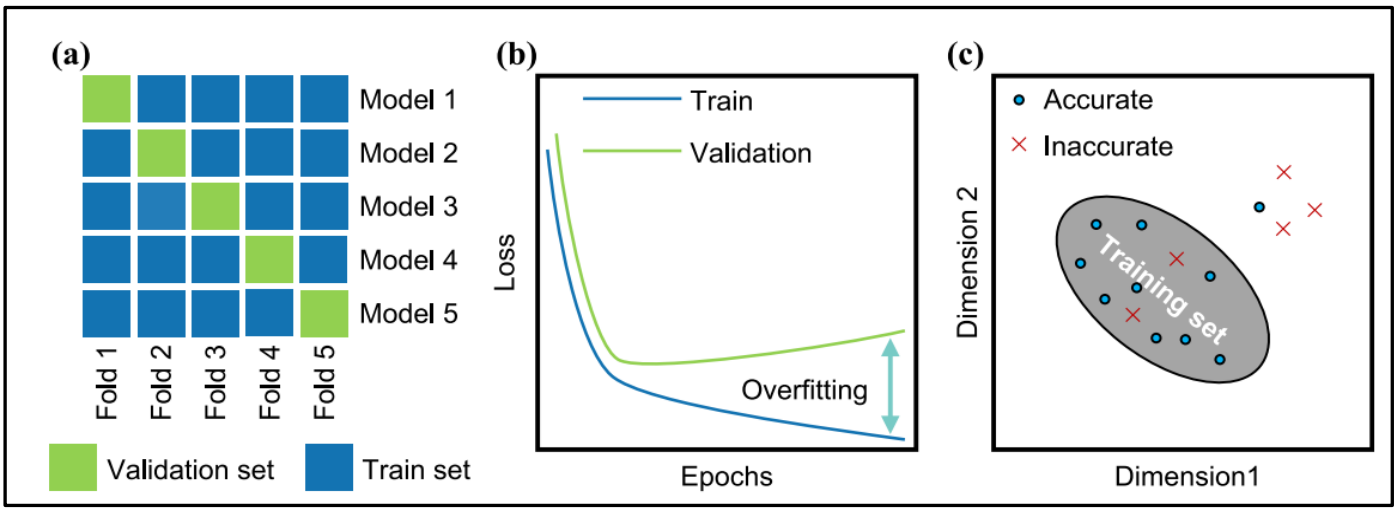

Fig 2 Schematic Representation of (a) 5-Fold Cross-Validation, (b) Overfitting, and (c) Accurate Prediction Region [9].

However, during training, overfitting arises when the model captures excessive details, including noise, from the training set, yet struggles to generalize to the validation or test set. For instance, in a neural network model, overfitting manifests as a continuous decrease in training loss accompanied by an increase in validation loss. Therefore, it is crucial to assess model performance using the test (validation) set [9]. Fig. 2 illustrates cross-validation, overfitting, and prediction accuracy regions.

➢ *Unsupervised ML in Ceramic Materials*

Unsupervised ML is a type of ML where the algorithm learns patterns, structures, or relationships from unlabeled data, meaning there are no predefined outputs or target values. In the context of ceramic materials research, unsupervised ML is particularly useful for exploring large datasets to identify trends, similar group compositions, or detect hidden correlations between processing parameters, microstructure features, and material properties. Common applications include clustering ceramic compositions with

comparable mechanical, thermal, or electrical behavior, and dimensionality reduction techniques like principal component analysis (PCA) to simplify complex microstructural or compositional datasets for visualization and analysis. By uncovering intrinsic patterns in data without human bias, unsupervised ML enables researchers to generate hypotheses, discover new material families, and guide experimental design more efficiently, complementing traditional supervised learning approaches in ceramics development.

- *Semi-supervised ML in Ceramic Materials*

Semi-supervised ML combines elements of supervised and unsupervised learning, leveraging a small amount of labeled data alongside a larger set of unlabeled data. In ceramic materials research, this approach is particularly useful because high-quality experimental datasets are often limited or expensive to obtain. Semi-supervised ML can improve predictions of properties such as hardness, thermal conductivity, or dielectric behavior by learning from both labeled measurements and unlabeled compositions or microstructures. It also aids in microstructure classification, defect detection, and phase identification, where only partial annotations are available. By maximizing the value of scarce labeled data while extracting patterns from unlabeled datasets, semi-supervised ML accelerates the design, optimization, and discovery of advanced ceramics, bridging the gap between data availability and predictive performance.

- *Reinforcement Learning (RL) in Ceramic Materials*

Reinforcement learning (RL) is a type of ML in which an algorithm learns to make decisions by interacting with an environment and receiving feedback in the form of rewards or penalties. In the context of ceramic materials research, RL is particularly promising for process optimization and autonomous experimentation. For example, it can be used to design adaptive sintering schedules, optimize machining or additive manufacturing parameters, and control multi-step fabrication processes to achieve desired microstructures and material properties. By continuously learning from outcomes, RL enables the system to identify optimal strategies in complex, high-dimensional processing spaces where traditional trial-and-error approaches are inefficient. This capability accelerates experimental workflows, reduces material waste, and enhances the reproducibility and performance of advanced ceramic materials.

III. ML MODELS APPLIED IN CERAMICS FROM LITERATURE

Table 1 summarizes the literature where ML models are used to design ceramics. Here, properties like single-phase probability and mechanical properties serve as labels to steer the training procedure.

Table 1 ML Models Used to Design Ceramics (Jun Zhang, 2023)

Year	Model Type	Training Dataset Size	Prediction Dataset Size	Fitting Target	Core Architecture*	Model Performance*	Ref
2025	PCA + K-means clustering	118	1342	Coefficient of thermal expansion (CTE)	PCA, K-means clustering, regression	Thermal Conductivity: reduced by 10–30%	[10]
2025	Regression	353	150,000	Thermal Conductivity	XGBoost (after comparing BG, RF, SVR, KRR, LR)	Training R^2 = 0.999, Test R^2 = 0.928, Test MSE = 0.00440	[11]
2025	Regression	164	30% of the dataset	Quality factor (Qf) values	SVR-rbf	Overall: R^2 = 0.65, RMSE =13,320 GHz	[12]
2025	Regression	60	20% split for test sets	Density and Hardness (HV)	XGBoost, BR, SR	Best model = Bagging Regression (BR): Prediction errors: 3.38% (density), 4.97% (hardness)	[13]
2024	Regression	Dataset I :114 Dataset II: 154	30% split for test sets	Phase transition temperatures (TC, TOT), Dielectric temperature spectrum	Scikit-learn with SVR-rbf, XGBoost, Random Forest	SVR-rbf: R^2 = 0.96 (TC), R^2 = 0.90 (TOT) XGBoost: MAE ≈ 8.1 °C	[14]
2024	Regression	56	210	EFA	SISSO	SISSO consistently outperformed KNN, SVR, and RF	[15]

2024	Regression	92	20% test split	Bulk density	LR, RF, LGBM	RF: R^2 = 0.923, RMSE = 0.166 g·cm^{-3} LGBM: R^2 = 0.596, RMSE = 0.379 g·cm^{-3} LR: R^2 = 0.226, RMSE = 0.525 g·cm^{-3}	[16]
2024	Regression	30,083	10% test	Total energy, atomic forces, virial stresses	DeePMD-kit NN	Elastic constants within 5–10% error vs. DFT; EOS matched up to ~30% strain Melting point = 1900 ± 50 K Hugoniot Elastic Limit (HEL) = 67 GPa	[17]
2024	Regression	150	80% train (~120 samples), 20% test (~30 samples)	Vickers hardness	Scikit-learn, XGBoost regressor	XGBoost: R^2 = 0.897, RMSE = 1.639 GPa, MAE = 1.151 GPa, MSE = 2.687 Gradient Boosting: R^2 = 0.819, RMSE = 2.172 GPa, MAE = 1.724	[18]
2023	Regression	1280	unknown	Carbon vacancy, Formation energy	RF	Test MAE: 0.054 eV	[19]
2023	Regression	167	252	Hardness	RF	RMSE: 2.3 GPa R^2: 0.92	[20]
2023	Regression	177	230,230	Young's modulus , Hardness	RF,SVR,ANN	R^2 > 0.92 for all.	[21]
2022	Regression	557	9212112	Hardness	RF, GBRT, DT	$(R^2)_{avg}$: 0.907	[22]
2022	Classification	126	unknown	Single-phase formability	KNN, LR, GNB	Test accuracy: ~94 %	[23]
2022	Regression	191	3.1M possible compositions	Piezoelectric coefficient (d_{33})	SVR	Training R^2 = 0.93 (SVR-rbf, 4 descriptors) Predicted d_{33} = 633 ± 70 pC/N Experimental d_{33} = 605 ± 14 pC/N Piezocatalytic degradation: 93% RhB in 100 min	[24]
2022	Classification	53	90	HECCs	ANN, SVM	ANN accuracy: 0.982, AUC: 0.956; SVM accuracy: 0.944, AUC: 0.940	[25]
2022	Regression	841	25	Contact angle of liquid metals and oxide ceramics	Linear regression variants	Test MAE ≈ 8–12, RMSE ≈ 10–15, R^2 < 0.90	[26]
2021	Regression	325	43494	Elastic moduli	GPR	Average MAE: 20 GPa	[27]

2021	Regression	438	436,494	Mechanical properties	Machine-learning regression with bond-parameter descriptors	Training dataset: 438 (DFT cases) Prediction space: ~436k ceramics Best model = GPR (exponential kernel) $R^2 \approx 0.95$ (Young's, Bulk moduli) Errors <10%;	[28]
2020	Regression	56	70	EFA	RF	Cr-containing HEEC: 7.0 (eV/ atom)-1; Train MAE: 3.8 (eV/ atom)-1	[29]

*RF: Random Forest; GBRT: Gradient Boosting Regression Trees; DT: Decision Tree, KNN: K-Nearest Neighbor; LR: Logistic Regression; GNB: Gaussian Naive Bayes; GPR: Gaussian Process Regression, MAE: Mean Absolute Error.

In addition, the crystal graph shown in fig. 3, the approach is applied to graph neural networks, where molecules and crystals are represented as graphs, atoms are nodes, and connections between atoms are edges. Each node and edge is assigned a vector to represent the properties of the atoms and bonds in the crystal [30]. In this article, the authors used this method to develop a graph deep learning energy model, which helps avoid the expensive calculations involved in structural relaxation using Density Functional Theory (DFT). They achieved a Mean Absolute Error (MAE) in energy prediction [31].

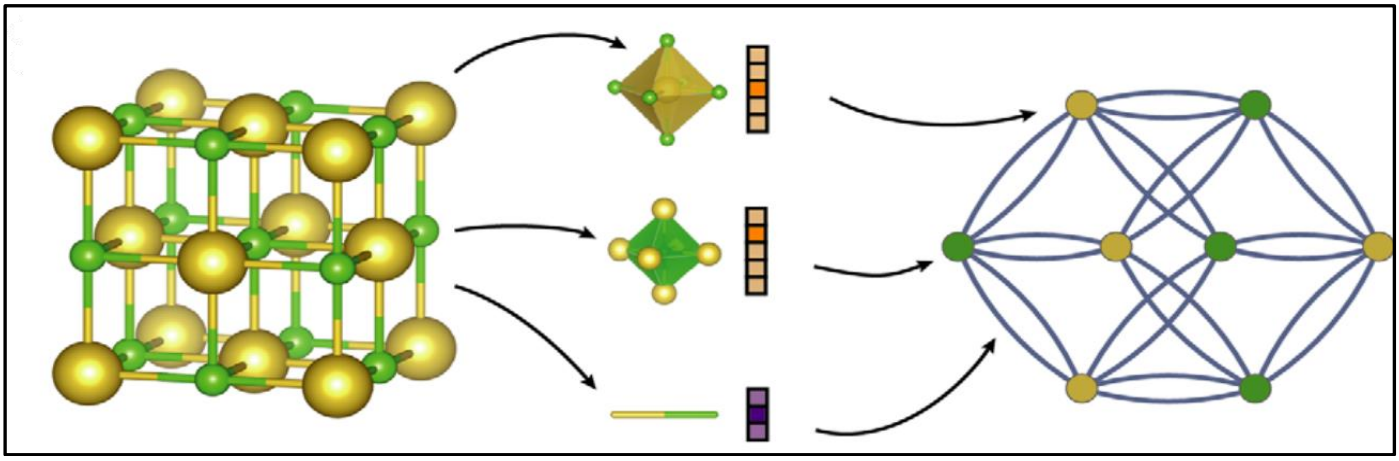

Fig 3 Illustration of Crystal Graph [30]

Furthermore, the properties of ceramics are predicted using deep potential molecular dynamics (DPMD) in fig.4. This method expresses the atomic energy as $E = \sum E_i$, where E_i and E stand for the atomic and total energies, respectively. Many-body interactions inside a cutoff distance (R_c) produce the energies. DPMD parses the coordinates with full (radial and angular) or radial information in order to maintain the geometrical symmetries (translation, rotation, and permutation).

Following this procedure, the atomic positions (R_i) are translated into descriptors (D_{ij}), which are then immediately inserted into neural networks. The authors predicted the thermal and mechanical properties of ceramics using the well-trained interatomic potentials, which are difficult to replicate directly using ab initio calculations [2].

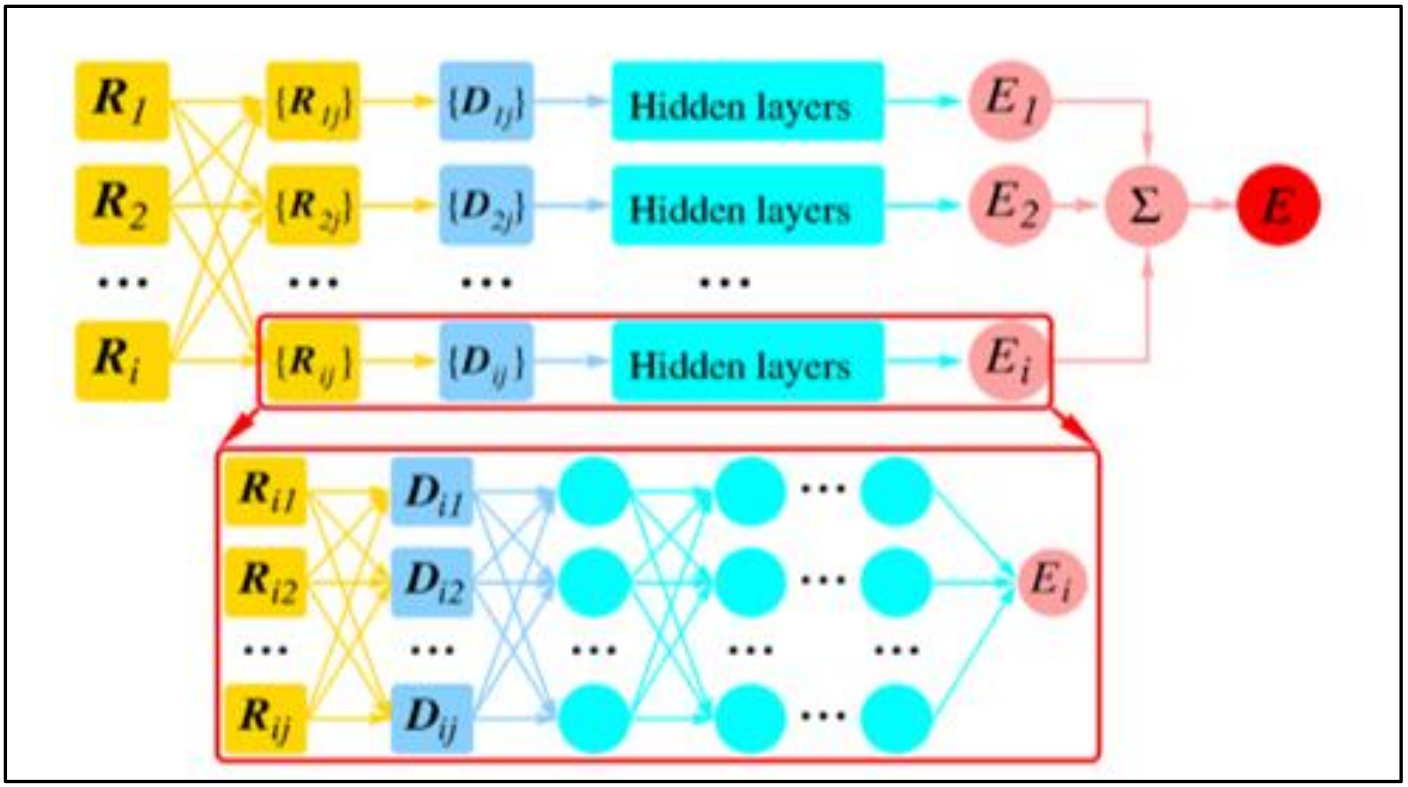

Fig 4 DPMD Model [2].

IV. CHALLENGES AND PROSPECTS OF ML IN CERAMIC MATERIALS

ML is being used more and more in ceramics because it can predict material properties and help find new ceramic materials faster and at lower cost than traditional experiments. ML can estimate properties like strength, hardness, thermal stability, and electrical behavior from the composition and structure of ceramics. It can also suggest new combinations of materials or processing methods that might perform better than current ones. However, there are still challenges. One major problem is the lack of large, high-quality datasets. Another issue is that predictions are sometimes not accurate enough, because ceramics have complex structures and behaviors that are hard to capture in a model.

To improve ML in ceramics, two strategies are especially important. First, researchers need to build large, reliable material databases. One way to do this is by using text mining, which collects data from published research papers, patents, and lab experiments. This would make it easier to gather scattered information and create specialized databases for ceramic materials. Second, ML methods themselves need to improve. Using better deep learning models and automating feature selection can help the model understand the relationships between composition, structure, processing, and properties more clearly. By combining these approaches, ML can become a powerful tool to design new ceramics, improve manufacturing processes, and speed up the discovery of high-performance materials.

V. CONCLUSION

ML holds great promise for predicting the behavior and properties of ceramics, including both the ability to synthesize single-phase materials and the prediction of mechanical, thermal, and functional properties. In recent years, there has been significant progress in applying ML to ceramics, and these advancements have been comprehensively reviewed in the literature. Key aspects covered include database acquisition, which involves gathering high-quality, structured data from experiments, publications, and simulations; input feature selection, which determines the most important material descriptors for accurate predictions; model selection, where different ML algorithms are tested for performance; and evaluation, which measures the reliability and accuracy of the predictions.

Several recent case studies have also been highlighted, showing how ML can successfully predict ceramic compositions, microstructures, and performance outcomes. At the same time, the field faces challenges that must be addressed to fully realize ML's potential in ceramics. Building large and reliable databases is crucial, as limited or inconsistent data can reduce model accuracy. Advances in deep learning techniques can help capture complex, nonlinear relationships between composition, processing, and properties. Label-free unsupervised learning offers a way to explore materials without requiring extensive labeled datasets, while high-throughput experimentation can accelerate data generation and model validation. Together, these strategies outline a clear roadmap for improving ML models for ceramics, enabling faster discovery, better process optimization, and more reliable design of high-performance materials.

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