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Advancements in Deep Learning for Materials Data Science: Applications across Atomistic, Imaging, Spectral, and Textual Data Modalities

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ABSTRACT: Deep learning (DL) has emerged as one of the most transformative technologies in materials data science, driven by its ability to process and analyze vast, complex datasets across various modalities. In recent years, DL has revolutionized how researchers handle atomistic, image-based, spectral, and textual data, automating feature identification and enabling more accurate predictions. This review provides an overview of deep learning methods in materials science, highlighting recent advancements in the field and the unique challenges associated with different data types. The rise of large-scale materials databases has propelled the use of DL in atomistic prediction, particularly for simulations at the atomic level. DL models have shown remarkable success in predicting material properties by learning from high-dimensional atomistic data, offering an efficient way to explore the structure-property relationship. In this domain, DL enables the automation of tasks traditionally requiring manual feature engineering, such as molecular dynamics simulations or quantum mechanical calculations. For image-based and spectral data, progress has been accelerated by the availability of synthetic data generated through high-fidelity forward models. DL techniques, particularly generative unsupervised models, have been employed to enhance image resolution, automate defect detection, and identify patterns in spectral data. In materials imaging, convolutional neural networks (CNNs) have proven especially useful, while auto encoders and other unsupervised models help reduce the complexity of spectral data for enhanced analysis. Natural language processing (NLP) in materials science is another rapidly advancing area. With the increasing availability of textual data, DL models such as recurrent neural networks (RNNs) and transformers have been applied to extract valuable information from scientific literature, patent filings, and experimental reports. This facilitates data mining and accelerates the discovery of new materials. The article also discusses cross-disciplinary work in uncertainty quantification, emphasizing the importance of understanding DL models' predictions in materials science. Additionally, the review highlights publicly available software tools and datasets that have supported these advancements, offering researchers easy access to resources for further exploration. Despite these advancements, challenges remain, such as the need for more interpretable models and overcoming data limitations. The article concludes by offering perspectives on future growth areas and potential challenges for deep learning applications in materials data science.

KEYWORDS: Deep Learning, Materials Data Science, Atomistic Prediction, Uncertainty Quantification

I. INTRODUCTION

The "Processing-Structure-Property-Performance" relationship is central to Materials Science and Engineering (MSE). The material structures and phenomena involved vary widely in length and time scales across these four elements, adding layers of complexity. For example, structural information can range from detailed atomic coordinates to the microscale spatial distribution of phases (microstructure), mesoscale fragment connectivity, and even images and spectra. Establishing connections between these components is a challenging endeavor.Both experimental and computational methods play crucial roles in identifying these relationships. The rapid advancement of automation in experimental equipment and the significant expansion of computational resources have led to an exponential increase in the size of public materials datasets. Numerous large experimental and computational datasets have been developed through initiatives like the Materials Genome Initiative (MGI) and the growing adoption of Findable, Accessible,

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Interoperable, Reusable (FAIR) principles. This data surge necessitates automated analysis, which can be efficiently achieved using machine learning (ML) techniques.

Deep learning (DL), a specialized branch of ML, was initially inspired by biological models of computation and cognition in the human brain. One of DL's key strengths lies in its ability to extract higher-level features from raw input data. DL applications are rapidly replacing conventional systems in many aspects of daily life, such as image and speech recognition, web search, fraud detection, email/spam filtering, and financial risk modeling. DL techniques have demonstrated exciting new capabilities in various fields, including playing Go, self-driving cars, navigation, chip design, particle physics, protein science, drug discovery, astrophysics, and object recognition. Recently, DL methods have been outperforming other machine learning techniques in numerous scientific disciplines, including chemistry, physics, biology, and materials science. Although DL applications in MSE are still relatively new, the field has yet to fully explore their potential, implications, and limitations. DL offers novel approaches for investigating material phenomena, prompting materials scientists to expand their traditional toolset.DL methods have proven to be a complementary approach to physics-based methods for materials design. While large datasets are often seen as necessary for successful DL applications, techniques such as transfer learning, multi-fidelity modeling, and active learning can make DL feasible even for small datasets.Traditionally, materials have been designed experimentally using trial-and-error methods combined with chemical intuition. However, this approach is both costly and time-consuming, and the vast number of material combinations makes it impractical to study experimentally. This has led to the need for empirical formulation and computational methods.

II. GENERAL MACHINE LEARNING CONCEPTS

This article does not aim to provide a detailed hands-on introduction to Deep Learning. For those interested in such resources, there are many available, including the free online book "Neural Networks and Deep Learning" by Michael Nielsen (http://neuralnetworksanddeeplearning.com), Deep Learning by Goodfellow et al., and various online courses on platforms like Coursera and Udemy. Instead, this article focuses on motivating materials scientists by highlighting the types of problems that are well-suited to DL and introducing some basic concepts, terminology, and relevant materials-specific databases and software (as of the time of writing) to facilitate getting started. To this end, we begin with a basic overview of Deep Learning.

Artificial Intelligence (AI) involves developing machines and algorithms that mimic human intelligence, such as by optimizing actions to achieve specific goals. Machine Learning (ML), a subset of AI, enables systems to learn from data without explicit programming, applicable to tasks like playing chess or making social network recommendations. Deep Learning (DL) is a further subset of ML, inspired by biological brains and utilizing multilayer neural networks to address ML tasks. Figure 1 provides a schematic of the AI-ML-DL context and highlights some key DL applications in materials science and engineering. Common ML techniques include linear regression, decision trees, and random forests, where generalized models learn coefficients, weights, or parameters from structured datasets (e.g., grids or spreadsheets). Applying traditional ML methods to unstructured data—such as pixels from images, sounds, text, or graphs—can be challenging, as users must first manually extract meaningful representations or features (e.g., calculating pair-distribution functions for atomic structures) before training the ML models. This process can be time-consuming, brittle, and not easily scalable, making deep learning (DL) techniques increasingly important.

III. NEURAL NETWORKS

3.1 Perceptron

A perceptron, or a single artificial neuron, is a fundamental component of artificial neural networks (ANNs) that facilitates the forward propagation of information. For a set of inputs [x1, x2, ..., xm] into the perceptron, floating-point weights [w1, w2, ..., wm] and biases are assigned, and these weights are multiplied with the inputs and summed to produce the output. Common software packages for training neural networks include PyTorch, TensorFlow, and MXNet. It is important to note that while certain commercial equipment, instruments, or materials are mentioned in this paper to describe the experimental procedure, this mention does not constitute a recommendation or endorsement by NIST, nor does it suggest that the identified materials or equipment are necessarily the best available for the purpose.

3.2 Activation function

Activation functions (such as sigmoid, hyperbolic tangent (tanh), rectified linear unit (ReLU), leaky ReLU, Swish) are the critical nonlinear components that enable neural networks to compose many small building blocks to learn complex nonlinear functions. For example, the sigmoid activation maps real numbers to the range (0, 1); this activation function

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is often used in the last layer of binary classifiers to model probabilities. The choice of activation function can affect training efficiency as well as final accuracy.

3.3 Loss function, gradient descent, and normalization

The weight matrices of a neural network are either initialized randomly or sourced from a pre-trained model. These weight matrices are multiplied by the input matrix (or the output from a previous layer) and passed through a nonlinear activation function to produce updated representations, commonly referred to as activations or feature maps. The loss function (also known as the objective function or empirical risk) is computed by comparing the neural network's output with the known target values. Typically, network weights are updated iteratively using stochastic gradient descent algorithms to minimize the loss function until the desired accuracy is reached. Most modern deep learning frameworks facilitate this process through reverse-mode automatic differentiation, which calculates the partial derivatives of the loss function with respect to each network parameter by recursively applying the chain rule, a method commonly known as back-propagation. Common gradient descent algorithms include Stochastic Gradient Descent (SGD), Adam, and Adagrad. The learning rate is a crucial parameter in gradient descent, with methods other than SGD using adaptive learning rate tuning. Depending on the task, such as classification or regression, different loss functions are utilized, including Binary Cross Entropy (BCE), Negative Log Likelihood (NLL), or Mean Squared Error (MSE). Inputs to a neural network are typically scaled, or normalized, to have zero mean and unit standard deviation. Scaling is also applied to the inputs of hidden layers, using techniques like batch or layer normalization, to enhance the stability of artificial neural networks (ANNs).

IV. DEEP REINFORCEMENT LEARNING

Reinforcement learning (RL) deals with tasks in which a computational agent learns to make decisions by trial and error. Deep RL uses DL into the RL framework, allowing agents to make decisions from unstructured input data79. In traditional RL, Markov decision process (MDP) is used in which an agent at every timestep takes action to receive a scalar reward and transitions to the next state according to system dynamics to learn policy in order to maximize returns. However, in deep RL, the states are high-dimensional (such as continuous images or spectra) which act as an input to DL methods. DRL architectures can be either model-based or model-free.

V. SCIENTIFIC MACHINE LEARNING

The emerging field of scientific machine learning (SciML) is creating new opportunities across all machine learning paradigms, with a particular focus on deep learning. SciML aims to develop machine learning systems that integrate scientific knowledge and physical principles, either directly within the model or indirectly through the optimization algorithms used during training. This approach has the potential to enhance sample and training efficiency, robustness (especially in extrapolation scenarios), and model interpretability. A notable theme in this area is discussed in reference 57, where multiple physics-based constraints are applied during the training of deep learning models.

One significant challenge with universal function approximation is that a neural network can quickly learn irrelevant features that are not of interest to researchers. In this context, physics-based regularization can be beneficial. Physics-based deep learning can also support inverse design problems, which are complex yet crucial tasks. Conversely, deep learning techniques such as Graph Neural Networks and symbolic regression (which involves stochastically constructing symbolic expressions) have been used to "discover" symbolic equations from data that reveal both known and unknown physical principles. This approach aims to develop a physics model through deep learning rather than constraining deep learning with existing physics models.

VI. IMAGE-BASED MODELS

Computer vision is often credited with sparking the current wave of mainstream deep learning applications a decade ago. As a result, materials researchers have developed a wide range of computer vision applications to enhance and accelerate image-based material characterization techniques. Key microscopy vision tasks include: image classification (and material property regression), auto-tuning experimental imaging hyperparameters, pixelwise learning (such as semantic segmentation), super-resolution imaging, object/entity recognition, localization, tracking, and microstructure representation learning. These tasks often generalize across various imaging modalities, including optical microscopy (OM), scanning electron microscopy (SEM), scanning probe microscopy (SPM) such as scanning tunneling microscopy (STM) or atomic force microscopy (AFM)—and transmission electron microscopy (TEM) variants, including scanning transmission electron microscopy (STEM).

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The images produced by these techniques capture a range of details from local atomic to mesoscale structures (microstructure), the distribution and types of defects, and their dynamics, which are crucial for understanding material functionality and performance. Atomic-scale imaging has become increasingly routine with the advent of aberration-corrected STEM. However, the growing volume of large image datasets is creating an analysis bottleneck in materials characterization, highlighting the need for automated image analysis. While non-deep learning image analysis methods have made significant strides in quantitative microscopy, these methods often rely on brittle image processing pipelines and excessive manual feature identification, limiting their broader applicability. Consequently, deep learning is now considered the most promising approach for high-performance, high-throughput automated analysis of image datasets. For a comprehensive overview of applications in microstructure characterization, see reference 210.

6.1 Image classification and regression

Classification and regression involve predicting one or more values associated with an image. In deep learning, the primary difference between these methods is that classification outputs discrete values, while regression models produce continuous values. The same network architecture can be used for both tasks by selecting the appropriate activation function for the output layer: a linear activation for regression and Softmax for classification. Despite its simplicity, image classification remains one of the most established deep learning techniques in the materials science literature and continues to be an area of active research.

Modarres et al. utilized deep learning with transfer learning to automatically classify SEM images of various material systems. They demonstrated that a single model could identify a range of features and material systems, including particles, fibers, Microelectromechanical Systems (MEMS) devices, and more, achieving 90% accuracy on a test set. Misclassifications were mainly due to images containing objects from multiple classes, a limitation inherent to single-class classification. More advanced techniques, discussed in later sections, can address these limitations. Additionally, they developed a system to deploy the trained model at scale, allowing for the parallel processing of thousands of images, which is crucial for large-scale, high-throughput experiments or industrial applications.Deep learning has also been successfully used for crack detection in macroscale materials images using ImageNet-based deep transfer learning and for property prediction on small, noisy, and heterogeneous industrial datasets.

Furthermore, deep learning has been applied to characterize symmetries in simulated measurements of samples. Ziletti et al. compiled a large database of perfect crystal structures, introduced defects into these lattices, and simulated diffraction patterns for each structure. They trained deep learning models to identify the space group of each diffraction pattern, achieving high classification performance even with significant defect presence, surpassing conventional algorithms for detecting symmetries from diffraction patterns.In another application, deep learning was used to classify symmetries in simulated STM measurements of 2D material systems. Using density functional theory (DFT), simulated STM images were generated for various material systems. A convolutional neural network was trained to identify which of the five 2D Bravais lattices each material belonged to, achieving an average F1 score of around 0.9 for each lattice type.

DL has also been used to improve the analysis of electron backscatter diffraction (EBSD) data, with Liu et al.218 presenting one of the first DL-based solution for EBSD indexing capable of taking an EBSD image as input and predicting the three Euler angles representing the orientation that would have led to the given EBSD pattern. However, they considered the three Euler angles to be independent of each other, creating separate CNNs for each angle, although the three angles should be considered together. Jha et al.219 built upon that work to train a single DL model to predict the three Euler angles in simulated EBSD patterns of polycrystalline Ni while directly minimizing the misorientation angle between the true and predicted orientations. When tested on experimental EBSD patterns, the model achieved 16% lower disorientation error than dictionary-based indexing. Similarly, Kaufman et al. trained a CNN to predict the corresponding space group for a given diffraction pattern220. This enables EBSD to be used for phase identification in samples where the existing phases are unknown, providing a faster or more costeffective method of characterizing than X-ray or neutron diffraction. The results from these studies demonstrate the promise of applying DL to improve the performance and utility of EBSD experiments. Recently, DL has also been to learn crystal plasticity using images of strain profiles as input221,222. The work in ref. 221 used domain knowledge integration in the form of two-point autocorrelation to enhance the predictive accuracy, while222 applied residual learning to learn crystal plasticity at nanoscale. It used strain profiles of materials of varying sample widths ranging from 2 μm down to 62.5 nm obtained from discrete dislocation dynamics to build a deep residual network capable of identifying prior deformation history of the sample as low, medium, or high. Compared to the correlation function-based method (68.24% accuracy), the DL model was found to be significantly more accurate (92.48%) and also capable of predicting stress-strain curves of test samples. This work additionally used saliency maps to try to interpret the developed DL model.

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6.2 Super-resolution imaging and auto-tuning experimental parameters

The studies mentioned so far focus on automating the analysis of existing data collected experimentally. However, deep learning (DL) can also be utilized during experiments to enhance data quality, reduce data collection time, or improve the amount of information captured in each image. DL techniques, such as super-resolution, can be applied in situ to autonomously adjust experimental parameters.

For instance, capturing high-resolution electron microscope images often requires long dwell times, which limits throughput. Additionally, interactions between the electron beam and the sample can lead to issues such as charging of non-conductive samples or damage to sensitive ones. DL can help address these issues by artificially increasing image resolution while minimizing artifacts. De Haan et al. used generative adversarial networks (GANs) to process low-resolution SEM images of carbon samples with gold nanoparticles, achieving a four-fold reduction in electron beam interaction time and improving image quality significantly.

Ede and Beanland employed GANs to reconstruct high-resolution STEM images from partial images obtained with reduced resolution, successfully reconstructing full images with minimal errors despite substantial subsampling. DL has also been applied to automate tip conditioning in scanning probe microscopy (SPM). Rashidi and Wolkow trained a model to detect artifacts from degraded tips, achieving 99% accuracy. The SPM was then set to automatically recondition the tip in situ until the network confirmed its restoration, thereby increasing throughput and reducing the labor and time required for tip maintenance. In manufacturing, DL can be used to adjust parameters during production. Scime et al. equipped multiple 3D printers with cameras to monitor the build plate throughout the printing process. A dynamic segmentation convolutional neural network was trained to detect defects such as recoater streaking, incomplete spreading, and spatter, achieving high performance across different printers and additive manufacturing methods. This work represents an initial step toward developing smart additive manufacturing machines capable of correcting defects and adjusting parameters in real-time.

Finally, there is growing interest in developing autonomous experimentation setups for laboratories. Eppel et al. trained multiple models to detect chemicals, materials, and transparent vessels in a chemistry lab. The study explored various approaches for scene understanding, including semantic and instance segmentation. While the models successfully identified vessels and materials, finer-grained analysis of multi-phase systems remains a challenge and highlights areas for future development. This research marks a significant advancement toward realizing fully automated laboratory-scale experiments.

VII. UNCERTAINTY QUANTIFICATION

Uncertainty quantification (UQ) is crucial for assessing the robustness of deep learning (DL) models. These models have been criticized for their lack of robustness, interpretability, and reliability, and incorporating carefully quantified uncertainties could help address these issues. While much of the current focus in the DL field is on developing new algorithms or achieving high training accuracy, there is growing interest in UQ, as highlighted by Abdar et al. However, quantifying uncertainty in DL predictions remains challenging and is far from a fully resolved issue. A major limitation is that most existing UQ methods are not applicable to arbitrary, off-the-shelf models without requiring retraining or redesign. Bayesian neural networks (NNs) are an exception but are computationally expensive and inefficient for large datasets. A significant portion of current research is dedicated to addressing this challenge: evaluating uncertainty without costly retraining or modifications to DL code. For example, Mi et al. explored scalable methods to assess the variance in outputs from trained NNs without retraining. Another approach by Teye, Azizpour, and Smith investigated using batch normalization to approximate inference in Bayesian models.

Before discussing common methods for evaluating uncertainty in DL, it is important to understand why adding UQ is beneficial. High accuracy in DL models typically presumes a large and diverse training dataset, which is often not available in material discovery applications. ML/DL models tend to perform poorly on extrapolation and struggle with ambiguous samples. Determining the necessary amount of training data for achieving desired accuracy is a complex problem. Evaluating uncertainty in DL predictions can enhance the reliability of results and guide decisions on the required dataset size and the addition of new data to reach target accuracy. Zhang, Kailkhura, and Han demonstrated that incorporating a UQ-driven reject option into DL models can significantly improve performance by detecting out-of-distribution samples through UQ analysis.

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Two main types of uncertainty are associated with ML predictions: epistemic and aleatory uncertainty. Epistemic uncertainty pertains to insufficient training data in certain parts of the input domain, affecting extrapolation accuracy. Aleatory uncertainty relates to factors not included in the model, such as missing features that cause the model to misinterpret similar data as having different outputs. Ideally, UQ methodologies should separately identify and quantify both types of uncertainties. Common approaches for evaluating uncertainty in DL include Dropout methods, Deep Ensemble methods, Quantile regression, and Gaussian Processes. Dropout methods are particularly well-known for helping to prevent overfitting.Deep ensemble methodologies combine deep learning with ensemble learning to enhance predictability. These methods use multiple models with different random initializations to generate a range of predictions, which form statistical distributions of outputs. By combining these predictions into a Gaussian distribution, confidence intervals can be derived through variance evaluation. This multi-model approach allows for the assessment of aleatory uncertainty when sufficient training data is available. In areas with limited data, the predicted mean and variance may not be accurate, but a large variance indicates unreliable predictions. Combining Monte-Carlo Dropout and Deep Ensembles can further improve confidence in predictions.

Gaussian Processes (GP) can also be integrated into deep learning approaches and offer the benefit of providing UQ information without additional cost. Gaussian processes are a class of infinite-dimensional multivariate Gaussian distributions defined by a mean function and a flexible kernel function (prior distribution). By optimizing these functions to fit training data, the posterior distribution is obtained, which is used to predict outputs for unseen inputs. The Gaussian nature of the prior and posterior distributions provides both mean and variance information for predictions. However, standard kernels often underperform. In 2016, Wilson et al. proposed processing inputs through a neural network before applying a Gaussian process model to capture high-level patterns and features, though this requires careful design and optimization. Deep Gaussian processes enhance performance by mapping inputs through multiple Gaussian process layers. Several researchers have refined this approach, but a common drawback of Bayesian methods is the high computational cost associated with large datasets.

VIII. LIMITATIONS AND CHALLENGES

Although deep learning (DL) methods offer significant potential for materials design, several limitations and areas for improvement persist. One major challenge is the reliability and quality assessment of datasets used in DL tasks. Issues arise from a lack of ground truth data, insufficient metrics for global comparison, and reproducibility concerns when datasets use similar or identical setups. These factors complicate the reliance on DL-based predictions.Material representations based solely on chemical formulas do not consider the structural details of materials. While this approach can be beneficial for new compounds with unknown structures, it fails to capture phenomena like phase transitions. The properties of materials are highly sensitive to their atomic arrangements, as evidenced by the stark differences between diamond (a hard, wide-band-gap insulator) and graphite (a soft, semi-metal). Consequently, chemical formula-based methods may not always be adequate.

Atomistic graph-based predictions, which offer a more detailed description, are often tested only on bulk materials and may not account for defective systems or multi-dimensional phase spaces explored by methods like genetic algorithms. This highlights the necessity for input features to be fully predictive of output labels. Although atomistic graph neural network models like the Atomistic Line Graph Neural Network (ALIGNN) have shown improved accuracy, model errors still need reduction to approach deep learning "chemical-accuracies."In the realm of images and spectra, experimental data are frequently noisy and require significant preprocessing before applying DL. Simulated data, while a viable alternative, may not accurately represent real-world scenarios, such as structured noise.Uncertainty quantification (UQ) in DL for materials science remains an underexplored area. Efforts like GNNExplainer aim to address the black-box nature of DL methods and improve interpretability. These advances are crucial for gaining the trust of the materials science community.

Traditional training-validation-test split strategies, designed for image classification with specific class numbers, may not be optimal for regression models in materials science. Models might encounter materials similar to those in the test set during training, complicating generalization. Developing best practices for data splitting, normalization, and augmentation is necessary to address these issues.A significant technological challenge is the creation of a closed-loop autonomous materials design and synthesis process that integrates both machine learning and experimental components. Early proof-of-principle experiments, such as those involving automatic adjustment of gas composition based on prior experiments, demonstrate the potential for fully autonomous systems. This represents an initial step toward the future of self-driving laboratories, highlighting the ongoing advancements and possibilities in this field.

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IX. CONCLUSION

Deep Learning (DL) has made significant strides in the field of materials data science, offering transformative solutions across multiple data modalities, including atomistic, imaging, spectral, and textual data. By automating feature extraction and enabling the analysis of unstructured data, DL has reshaped how materials scientists approach complex problems, leading to breakthroughs in material discovery and characterization. In atomistic simulations, DL models have shown exceptional capability in predicting material properties, reducing reliance on traditional, computationally expensive methods. The availability of large materials databases has further fueled this progress, allowing DL to become a key tool in atomistic prediction. In the domains of materials imaging and spectral analysis, DL has also made considerable advancements. Generative unsupervised learning and high-fidelity forward models have allowed researchers to work with synthetic data to improve image resolution, automate defect detection and analyze complex spectral patterns. These applications underscore the versatility of DL in processing diverse types of scientific data. Additionally, DL models for natural language processing (NLP) have become powerful tools for extracting valuable insights from the vast textual resources in the form of scientific literature and patents, accelerating innovation and material discovery. Despite these achievements, several challenges persist, including the need for more interpretable models, better integration of experimental and theoretical data, and advancements in uncertainty quantification. Addressing these challenges will be crucial for the further growth of DL in materials science. Looking ahead, cross-disciplinary collaboration and the development of publicly available datasets and software will continue to support the evolution of DL applications in this field. As materials science becomes increasingly data-driven, the potential for DL to drive innovation and enhance understanding of complex materials systems will only grow, offering exciting possibilities for future research and development.

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