

Physics-Informed AI for Material Characterization: A Perspective on Data-Efficient Discovery through Physics-Informed Neural Networks

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Abstract

Accurate characterization of material properties is critical for modeling and optimizing advanced systems, yet conventional experimental and simulation-based approaches remain costly and data-intensive. As artificial intelligence (AI) evolves from data-driven modeling to physics-informed and knowledge-guided paradigms, this Perspective highlights the role of physics-informed machine learning (PIML), specifically physics-informed neural networks (PINNs), as a key enabler of data-efficient, physically consistent inference. PINNs embed governing equations into the learning process and have demonstrated strong capability in recovering constitutive and transport parameters from sparse or noisy data while preserving physical fidelity. This Perspective examines the fundamental structure, workflow integration, and recent advances of PINNs in the context of inverse material characterization. It also discusses open challenges in computational cost, training stability, and uncertainty quantification. Looking forward, integration with digital twins, generative modeling, and autonomous experimentation presents a pathway toward interpretable, adaptive, and automated characterization for next-generation intelligent manufacturing.

1. Introduction

The rapid advancement of artificial intelligence (AI) and machine learning (ML) has profoundly transformed modern engineering. A clear trajectory has emerged toward knowledge-guided AI, where learning is informed not only by data but also by embedded physical principles and domain expertise ^[1]. The early phase of AI integration was primarily driven by data-driven surrogate modeling, where large datasets were utilized to approximate complex physical responses without explicitly incorporating governing physical laws ^[2-6]. This paradigm subsequently evolved toward generative modeling, in which models approximate the underlying data distribution and generate novel, distribution-consistent samples rather than memorized replicas of the training data ^[7,8]. It has further advanced into the realm of physics-informed machine learning (PIML), which integrates governing equations and physical constraints directly into the learning process ^[9,10]. More recently, the emergence of large language models (LLMs) and agentic AI systems has accelerated this transformation by introducing autonomous reasoning, adaptive model construction, and closed-loop experimentation into engineering workflows ^[11-13], as summarized in **Table 1**. Within this overarching framework of knowledge-guided AI, this Perspective represents the physics-knowledge-guided component, focusing on the physics-informed foundation through PIML and its core formulation, physics-informed neural networks (PINNs). As summarized in **Fig. 1**, PIML encompasses several frameworks, including feature-augmented models, invariant and equivariant networks, physics-informed neural networks (PINNs), and operator learning methods ^[9,14,15]. Among these, this Perspective focuses on PINNs as a representative and widely adopted formulation that enables data-efficient, interpretable, and reliable characterization of material properties.

Such knowledge-guided transformation is particularly critical in material property

characterization, where purely data-driven approaches often fail to capture the underlying physics governing complex material behavior. Accurately identifying material properties, therefore, remains a persistent challenge in materials engineering and computational mechanics. Conventional experimental and numerical approaches—such as mechanical testing, curve fitting, or inverse finite element analysis—typically require extensive data, substantial computational resources, and significant domain expertise ^[16,17]. These limitations are further exacerbated for nonlinear, anisotropic, or coupled multi-physics systems, where replicating realistic boundary and environmental conditions is inherently difficult and measurement data are often sparse or noisy. Although machine learning-based surrogates can accelerate parameter estimation, they generally depend on large datasets and often lose physical interpretability, leading to limited generalization ^[18-20].

To address these challenges, PINNs combine physical laws with data-driven learning in a unified framework that enables parameter identification under limited or uncertain data conditions while maintaining consistency with governing equations ^[21-23]. This Perspective provides a concise overview of the current status and emerging challenges in material property characterization, highlighting how conventional experimental, numerical, and data-driven approaches can be further complemented by physics-informed learning. In this context, physics-informed neural networks (PINNs) are discussed as a promising framework that bridges physical modeling and machine learning to enable data-efficient, interpretable, and reliable inference of material properties. The general framework of PINNs for material property identification is then outlined, followed by discussions on representative applications, remaining technical challenges, and future opportunities for integrating physics-informed AI into digital-twin and AI-driven manufacturing environments.

2. Current status and challenges

While the importance of accurate material characterization is widely recognized, achieving it in practice remains challenging due to technical and methodological limitations. Traditional inverse modeling approaches such as curve fitting, finite element–based parameter optimization, and surrogate-assisted regression have contributed significantly to the field, yet they often face limitations in computational cost, sensitivity to noise, and reliance on expert-driven trial-and-error procedures. These difficulties become more pronounced in nonlinear, anisotropic, or coupled multi-physics systems, where reproducing realistic loading and boundary conditions is inherently complex and experimental data are often sparse or uncertain.

In recent years, ML techniques have been explored as alternatives for accelerating material property identification. Methods such as neural networks, Gaussian process regression, and polynomial chaos expansion have been employed to correlate measured responses with underlying material parameters. These data-driven approaches can substantially reduce calibration time; however, their performance and generalization remain highly dependent on the quality and diversity of the available datasets. When data are limited, such models may suffer from overfitting and reduced generalization capability. Moreover, because physical constraints are often imposed externally rather than inherently embedded within the learning architecture, their interpretability and physical consistency can be difficult to maintain. On the other hand, physics-based inverse methods grounded in partial differential equation (PDE) formulations offer higher physical fidelity but remain computationally expensive and ill-posed, as multiple parameter sets can yield nearly identical responses. Even Bayesian inference, despite providing uncertainty quantification, can become computationally intractable for high-dimensional systems.

Building on these developments, PINNs have emerged as a promising hybrid paradigm

that unifies data-driven learning and physics-based modeling. As illustrated in **Fig. 2**, a PINN provides a unified framework applicable to both forward and inverse problems. In the forward setting, the network predicts physical field responses that satisfy governing equations for given material parameters and boundary conditions, whereas in the inverse setting, it identifies unknown material parameters from sparse or noisy measurements while preserving physical consistency. This bidirectional capability highlights the versatility of PINNs for integrating experimental data and physical modeling within a single learning architecture. Through this formulation, PINNs bridge the gap between conventional physics-based simulation and modern AI-driven discovery, laying the foundation for data-efficient and interpretable material characterization.

3. Opportunities of PINNs for material property characterization

PINNs provide a unified learning framework that couples experimental data with governing physical equations, enabling data-efficient and physically consistent inference of material properties. Unlike conventional data-driven neural networks that rely solely on large labeled datasets, they integrate physics-based loss functions derived from the governing equations of material behavior. This formulation allows the network to infer both field variables and constitutive parameters while automatically enforcing equilibrium, compatibility, and boundary conditions. The total loss function comprises two components: a data term that minimizes the difference between network predictions and available measurements, and a physics term that penalizes deviations from the governing equations. By jointly minimizing these terms, the model can learn physically admissible solutions even when data are sparse or noisy.

To better illustrate this concept, **Fig. 3** compares the conventional data-driven and physics-informed approaches for material property characterization. In the conventional approach, a neural network is trained on direct datasets such as stress–strain (σ, ε) pairs, which restricts its applicability to the training range and often results in non-physical extrapolation. In contrast, the physics-informed approach combines both direct and indirect data, such as displacement–force (u, F) measurements, with physical constraints and domain knowledge. By embedding this information into the training process, PINNs learn not only the mapping between inputs and outputs but also the underlying physical relationships. As shown in **Fig. 3**, the conventional model fits the training data but diverges under unobserved conditions, whereas the physics-informed model maintains physically meaningful responses beyond the observed range. This capability makes PINNs particularly suitable for inverse material characterization, where experimental data are limited but the underlying physics is well

established.

Beyond single-physics problems, the framework can be readily extended to multi-physics systems such as thermo-mechanical, electro-mechanical, or flexoelectric materials by incorporating the corresponding governing equations into the physics-based loss term. This flexibility enables cross-domain inference, where different physical fields are coupled within a single learning framework. For instance, in thermoelectric systems, voltage measurements can be leveraged to infer thermal conductivity, allowing efficient estimation of transport properties without direct thermal measurements. Recent developments have further introduced Bayesian formulations of PINNs, which provide probabilistic uncertainty quantification and enhance robustness against sensor noise and incomplete data ^[24]. Such approaches extend the applicability of PINNs to real experimental settings while maintaining physical consistency and interpretability. Collectively, these capabilities position PINNs as a practical and robust tool for data-efficient, physics-consistent identification of material properties, bridging the gap between traditional inverse modeling and modern AI-driven materials design. The specific applications of this framework are discussed in **Section 4**.

4. PINN-based material characterization workflow

Recent advances have demonstrated that PINNs can be systematically integrated into the overall workflow of material property characterization, bridging experimental measurement, data processing, constitutive modeling, and computational validation. As illustrated in **Fig. 4**, this workflow consists of five key stages: (a) material testing and data acquisition, (b) dataset construction and pre-processing, (c) constitutive relation modeling, (d) PINN-based material characterization, and (e) validation via finite-element simulations. This end-to-end framework highlights how physics-informed learning can unify experimental and computational mechanics within a single, data-efficient process.

In stage (a), mechanical experiments such as uniaxial or multiaxial tests generate displacement, strain, and force data, often supported by digital image correlation (DIC) for full-field measurements. These observations, organized in stage (b), are structured into datasets that combine direct and indirect quantities, forming the foundation for data-driven inference. Stage (c) addresses constitutive modeling, where the material response—traditionally expressed by analytical functions of stress and strain—is replaced or augmented by a neural representation. The parameters of this neural constitutive model become trainable variables within the physics-informed framework.

Stage (d) represents the core of the workflow: the PINN formulation. Here, governing PDEs, boundary conditions, and measurement data are simultaneously embedded into a unified loss function composed of data and physics terms. The network learns latent constitutive behavior and field distributions consistent with both observations and physical laws. Depending on the problem, the governing equations can be implemented in strong, weak, or energy forms and combined with diverse training strategies such as finite-difference, finite-element, or time-marching schemes. Stage (e) validates the inferred model through FEM or

other high-fidelity solvers. The discovered material parameters or learned constitutive relations are substituted into forward simulations and compared with experimental data to assess accuracy and generalization. Agreement among experiments, FEM, and PINN predictions confirms the reliability of the inferred models.

Although **Fig. 4** illustrates a representative workflow for mechanical property identification, the same formulation is readily extendable to other material properties and coupled multi-physics systems. By incorporating additional governing equations (e.g., energy or charge balance), the framework can be applied to thermal, electrical, and thermoelectric materials, as well as magneto-mechanical and flexoelectric systems ^[25-27]. This generality underscores the versatility of PINNs as a unifying tool for physics-based characterization of properties across diverse material classes. Overall, this integrated workflow demonstrates how PINNs can serve as the computational backbone of modern materials research. By connecting laboratory measurements with data-driven constitutive modeling and simulation-based verification, PINNs enable autonomous, closed-loop characterization frameworks that are essential for digital-twin and AI-driven manufacturing systems.

5. Future directions and outlook

Despite rapid progress, several key challenges remain before PINNs can be established as a reliable and widely adopted tool for materials characterization. The highest priority is establishing benchmark datasets that encompass diverse material systems, including elastic, thermal, electrical, and damage-sensitive materials, to ensure fair comparisons and reproducibility across studies. Equally important is integrating robust uncertainty quantification (UQ). Bayesian and probabilistic variants of PINNs offer a route to quantify predictive confidence and account for measurement noise, which is essential given the framework's high sensitivity to data quality, where sparse or biased measurements can lead to non-unique or unstable solutions.

On the methodological aspect, developing robust training strategies for multi-scale and multi-physics problems is critical. While recent advances such as Fourier feature embeddings and adaptive loss balancing show promise, the computational cost remains a major barrier, particularly for three-dimensional systems that require repeated differentiation of complex PDE operators. Moreover, model design choices, including the selection of governing equations, network architectures, and loss formulations, are still problem-dependent and lack standardized best practices. Perhaps, the most significant challenge is extending PINNs to nonlinear, history-dependent materials, such as those exhibiting plasticity, viscoelasticity, or fracture, due to their dependence on internal state variables and loading paths. Furthermore, the interpretability of the learned latent representations is an ongoing issue, as it is often unclear how physical meaning is encoded within the network's internal features.

Looking forward, the next generation of physics-informed AI is expected to move beyond the classical PINN formulation toward hybrid, interpretable, and generative frameworks. Integrating generative modeling principles could alleviate the ill-posedness

inherent in inverse problems, providing probabilistic descriptions of admissible material parameters rather than single deterministic estimates. Meanwhile, LLMs and knowledge-augmented networks may further enrich physical priors and assist in model design through embedded domain expertise. Ultimately, the goal is to achieve reliable, data-efficient, and autonomous material characterization—a paradigm in which models not only learn from data and physics but also reason about uncertainty, adapt across material classes, and interact seamlessly with experimental and computational platforms. Realizing this vision will establish physics-informed AI as a cornerstone of next-generation materials discovery and manufacturing.

6. Conclusion

The evolution of AI in materials science has advanced from purely data-driven modeling to generative, physics-informed, and ultimately knowledge-guided paradigms. Within this progression, PINNs represent a pivotal step toward unifying data and physics for reliable and data-efficient material characterization. By embedding governing equations and physical constraints directly into the learning process, PINNs enable the inference of constitutive and transport parameters even when experimental data are sparse, incomplete, or noisy. This integration of physical reasoning and machine learning has fundamentally reshaped the way materials are modeled, characterized, and designed.

Realizing the full potential of physics-informed AI, however, requires more than algorithmic innovation. The field must address challenges in data standardization, reproducibility, and computational scalability, while also developing robust frameworks for uncertainty quantification and interpretability. Collaborative efforts toward open benchmark datasets, standardized training protocols, and transparent evaluation metrics will be essential to ensure reliability and comparability across studies. Strengthening the integration between experimental and computational domains will further accelerate the transition from proof-of-concept demonstrations to practical engineering applications.

Looking forward, physics-informed AI is expected to evolve into hybrid and autonomous paradigms that combine the interpretability of physics with the adaptability of data-driven learning. Generative modeling principles, probabilistic inference, and knowledge-augmented architectures—potentially guided by LLMs—will further enhance physical understanding and enable intelligent design exploration. Ultimately, this convergence of physics, data, and intelligence is poised to transform materials research into a self-adaptive, closed-loop ecosystem capable of reasoning, learning, and discovery.

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Conflict of interest

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Table 1. Summary of key AI paradigms, their implications and limitations

Category	Representative Models	Implications	Limitations
Data-driven surrogate modeling	GPR, CNN, LSTM	Enables accelerated simulation modeling and efficient design optimization using simulation-derived data.	Strong data dependence; poor extrapolation; lacks physical interpretability.
Generative AI	VAE, GAN, Diffusion models	Supports data augmentation and exploration of complex design spaces for materials and structures.	Restricted by training distribution; no explicit physical constraints.
Physics-informed machine learning (PIML)	PINNs, physics-informed neural operators, physics-constrained nets	Integrates governing equations into learning; improves data efficiency and physical consistency.	High computational cost; sensitivity to data quality; limited standardization.
Agentic AI	LLM-based tool-using agents, multi-agent systems	Enables autonomous experiment planning and knowledge-driven reasoning across workflows.	Complex implementation; limited real-time reasoning and interpretability.

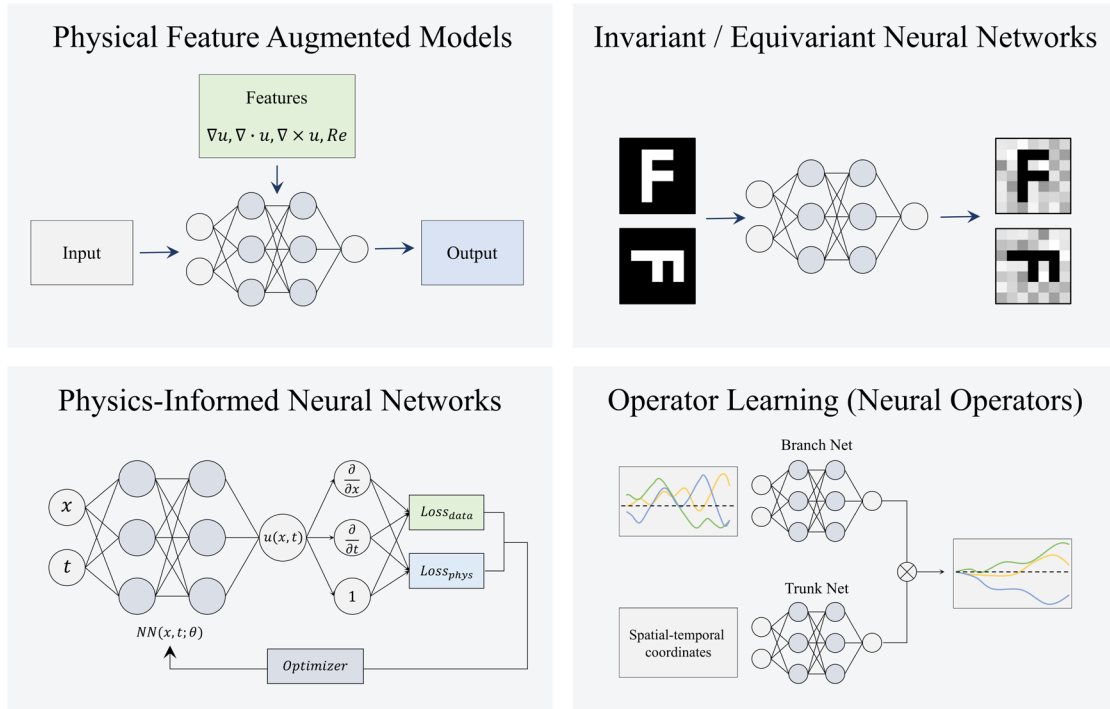


Fig. 1. Four Representative Frameworks in Physics-Informed Machine Learning. Four representative frameworks of PIML are illustrated, including physical feature-augmented models that explicitly incorporate user-defined physical descriptors such as gradients or dimensionless numbers, invariant and equivariant networks that enforce physical symmetries through architectural design, physics-informed neural networks that embed governing equations into the loss function, and operator learning frameworks that learn mappings between function spaces.

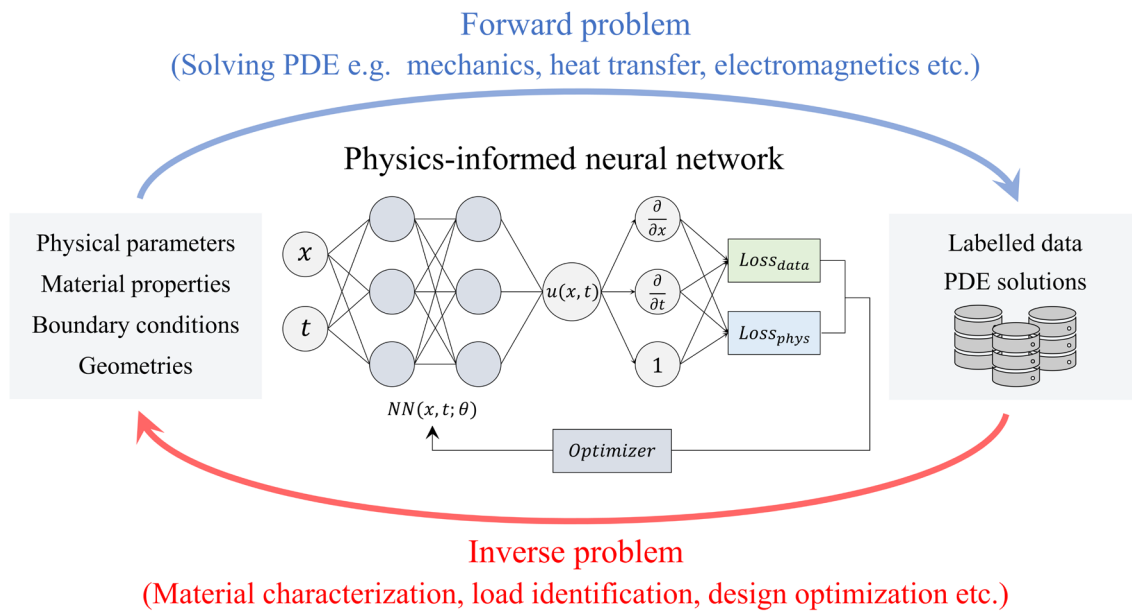


Fig. 2. Schematic illustration of a physics-informed neural network (PINN) for forward and inverse problems.

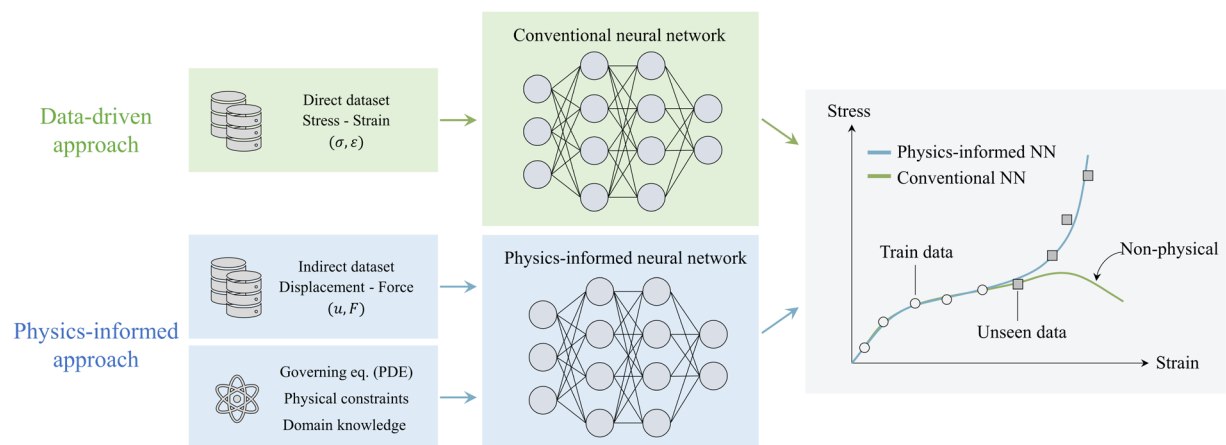


Fig. 3. Comparison of conventional neural networks and physics-informed neural networks (PINNs) for material property characterization.

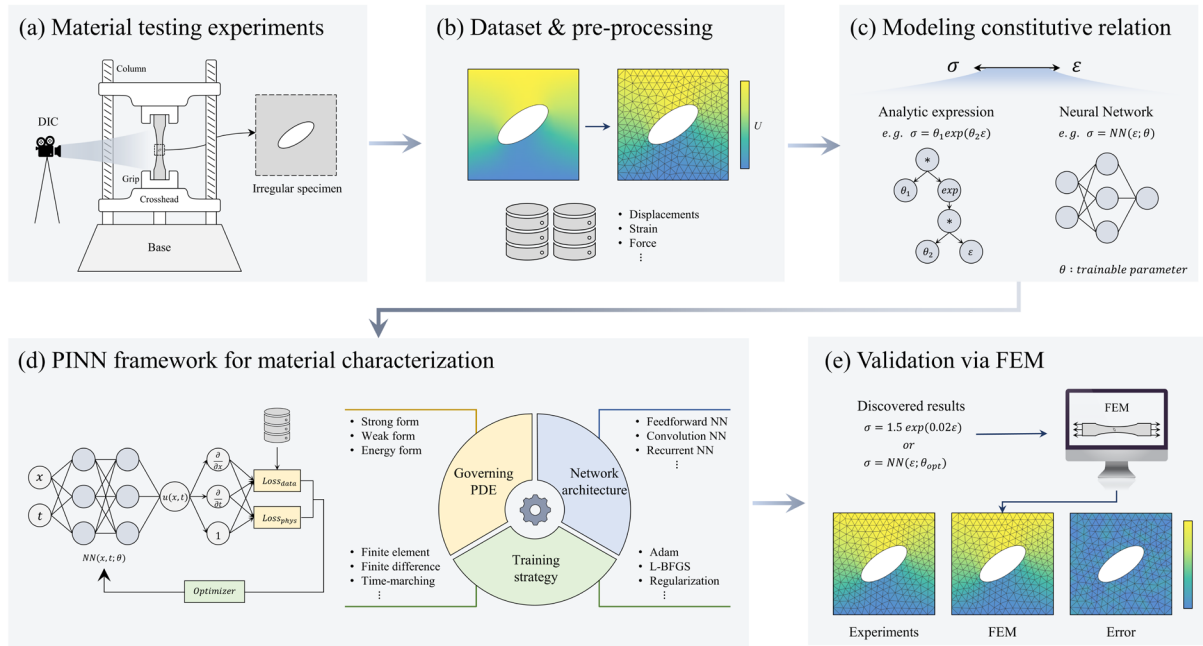


Fig. 4. Representative workflow of physics-informed neural networks (PINNs) for material characterization. (a) Material testing and data acquisition, (b) Dataset construction and pre-processing, (c) Constitutive relation modeling, (d) PINN-based material characterization integrating governing equations, network architecture, and training strategy, and (e) Validation via FEM simulations and experimental comparison.