

ORIGINAL RESEARCH

Open access

Physics-Constrained Neural Networks for Predicting Phase Transformation Pathways in Multi-Component Alloys

Wei Chen¹, Li Zhang^{1*}, Rui Zhao²

Abstract

Phase transformations in multi-component alloys underpin microstructural evolution and performance in advanced engineering systems. Yet, their prediction remains a persistent challenge due to the interplay of thermodynamic complexity, kinetic constraints, and sparse data regimes. While machine-learning approaches have shown promise in accelerating materials discovery, purely data-driven models often lack physical fidelity, interpretability, and robustness when extrapolated across high-dimensional compositional spaces. This paper introduces a conceptual framework for physics-constrained neural networks (PCNNs) to predict phase transformation pathways rather than static equilibrium states in multi-component alloy systems. The framework embeds thermodynamic and kinetic principles directly into the learning objective, reframing physical laws as epistemic constraints that govern admissible predictions. Unlike conventional physics-informed neural networks that solve predefined equations, the proposed approach integrates higher-level physical criteria—such as Gibbs free-energy minimization, phase coexistence rules, and diffusion-based kinetics—into a unified optimization logic. The contribution of this work is theoretical rather than empirical. By articulating how physical constraints regularize learning, enhance interpretability, and support generalization under data scarcity, the framework advances applied artificial intelligence as a decision-relevant modeling paradigm for materials science. Implications for alloy design, model trustworthiness, and AI-assisted exploration of complex phase spaces are discussed.

Keywords Materials design, Physics-constrained neural networks, Phase transformations, Multi-component alloys, Thermodynamic constraints, Kinetic modeling

*Correspondence:

Li Zhang

li.zhang@outlook.com

¹ Department of Computational Materials Science, School of Materials Engineering, Tsinghua University, Beijing, China

² Department of Artificial Intelligence and Data Analytics, Faculty of Computer Science, Peking University, Beijing, China

Introduction

Motivation: AI, complexity, and phase transformations

The development of advanced materials with tailored, reliable properties remains a central challenge in modern engineering, particularly in aerospace, automotive, nuclear, and energy systems, where materials operate under extreme mechanical, thermal, and chemical conditions. Within this landscape, multi-component alloys—including high-entropy alloys (HEAs) and complex concentrated alloys (CCAs)—have emerged as a high-impact class of materials due to their exceptional combinations of strength, ductility, corrosion resistance, irradiation tolerance, and thermal stability [1, 2]. Unlike conventional binary or ternary alloys, these systems explicitly leverage compositional complexity as a design variable, opening vast, largely unexplored material design spaces.

Central to the performance of multi-component alloys are phase transformations, which govern microstructural evolution during solidification, thermomechanical processing, and in-service operation. These transformations are therefore decision-critical phenomena, directly shaping macroscopic properties and long-term reliability. In multi-component systems, phase transformations proceed through intricate, path-dependent sequences of nucleation, growth, and dissolution, driven by competing thermodynamic forces and kinetic barriers. The simultaneous interaction of multiple alloying elements induces strong non-linearity, metastability, and history dependence, rendering transformation pathways highly sensitive to composition and processing conditions.

These characteristics expose fundamental limits of equilibrium-only reasoning. While equilibrium phase stability provides valuable insight, real alloy processing and service conditions are dominated by non-equilibrium kinetics, sluggish diffusion, and metastable phase retention. As a result, predictive frameworks that neglect transformation pathways in favor of static equilibrium states fail to support informed decision-making in alloy design and deployment.

Limitations of existing modeling paradigms

Historically, phase transformation modeling has relied on experimental characterization—such as differential scanning calorimetry, X-ray diffraction, and electron microscopy—alongside physics-based computational approaches, most notably the CALPHAD (Calculation of Phase Diagrams) methodology [3]. CALPHAD has proven indispensable for predicting equilibrium phase stability by minimizing Gibbs free energy across composition–temperature space. However, its effectiveness diminishes rapidly as system dimensionality increases. Multi-component alloys require extensive thermodynamic databases and parameter-optimization procedures that are costly, time-intensive, and often incomplete. Moreover, CALPHAD is intrinsically equilibrium-focused and usually decoupled from kinetic phenomena, such as diffusion-controlled transformations, nucleation delays, and non-equilibrium phase persistence, which dominate realistic processing conditions [4].

In parallel, advances in artificial intelligence (AI) and machine learning (ML) have introduced data-driven alternatives for modeling the behavior of complex materials. Neural networks and related ML architectures have demonstrated strong capabilities for learning high-dimensional, non-linear mappings between composition, processing variables, and material properties, accelerating alloy discovery and screening [5, 6]. In the context of phase stability and transformation prediction, ML models offer the appealing possibility of bypassing explicit thermodynamic modeling by inferring patterns directly from data.

However, purely data-driven approaches exhibit critical limitations in multi-component alloy systems. The combinatorial explosion of possible compositions leads to severe data sparsity, undermining statistical robustness. Unconstrained neural networks may also generate predictions that violate fundamental physical principles, such as thermodynamic stability or mass conservation, compromising scientific credibility. Furthermore, the black-box nature of many ML models limits interpretability, impeding mechanistic insight and eroding trust in predictions for high-stakes engineering applications.

Physics-informed neural networks (PINNs) have emerged as a hybrid response to these challenges by embedding governing physical laws—such as partial differential equations and conservation relations—into the learning process [7, 8]. Within materials science, PINNs have been applied to defect characterization, inverse property identification, and microstructure evolution, particularly in data-scarce regimes [9]. Nevertheless, most PINN implementations remain equation-centric and are primarily suited to continuous field prediction. Their application to phase transformation pathways, especially the ordered sequence and kinetics of phase evolution in multi-component alloys, remains limited.

Research gap

Despite substantial progress in both physics-based and data-driven modeling, a critical gap persists: the absence of a framework capable of predicting physically admissible phase transformation pathways in multi-component alloys under sparse-data conditions while remaining interpretable. Existing approaches either privilege equilibrium thermodynamics at

the expense of kinetics or rely on unconstrained statistical learning, which risks physical inconsistency and epistemic overreach. What is missing is a modeling paradigm that treats physical laws not merely as post hoc validation criteria, but as integral constraints shaping admissible AI predictions.

Contribution and scope

This manuscript addresses this gap by introducing a physics-constrained neural network (PCNN) framework as a conceptual applied artificial intelligence paradigm for predicting phase transformation pathways in multi-component alloys. Unlike conventional PINNs that focus on solving predefined field equations, the proposed framework integrates thermodynamic and kinetic principles at a higher epistemic level, embedding constraints such as Gibbs free energy minimization, phase stability criteria, the Gibbs phase rule, and diffusion-based kinetics directly into the learning objective.

The framework is explicitly pathway-oriented, emphasizing sequences of phase evolution rather than isolated equilibrium predictions. Importantly, this work is purely theoretical. No experiments, simulations, or datasets are introduced. Instead, the contribution lies in articulating a logically coherent and physically grounded AI framework that enhances generalizability, mitigates overfitting in sparse-data regimes, and improves interpretability by aligning network behavior with explicit physical mechanisms.

By uniting the flexibility of AI with the rigor of physical law, the proposed PCNN framework contributes to the broader evolution of applied artificial intelligence in materials science, with implications for sustainable alloy design, accelerated discovery, and informed decision-making in advanced engineering systems [10].

This theoretical positioning of the PCNN paradigm relative to established thermodynamic and data-driven modeling approaches motivates the comparative overview provided in Table 1.

Table 1. Comparison of conventional physics-based models, data-driven machine learning approaches, and the proposed physics-constrained neural network (PCNN) framework for predicting phase transformations in multi-component alloys

Modeling approach	Governing principle	Thermodynamics	Kinetics	Data dependence	Generalizability	Physical consistency	Interpretability
CALPHAD	Gibbs free energy minimization	Explicit	Limited/indirect	High	Moderate	High	High
Pure ML models	Statistical pattern learning	Implicit/none	Implicit/none	Very high	Low in sparse regimes	Low	Low
PINNs	PDE-constrained learning	Explicit (equation-based)	Explicit (equation-based)	Moderate	Moderate	High	Medium
Proposed PCNN	Physics-constrained optimization	Explicit (loss constraints)	Explicit (loss constraints)	Low to moderate	High	High	High

In the sections that follow, recent literature is synthesized to contextualize the evolution of machine learning in materials science and the growing role of physics-constrained approaches. The proposed conceptual framework is then articulated in detail, emphasizing its structure, assumptions, and theoretical propositions. As instructed, this manuscript concludes at the end of Part 1, establishing a clear theoretical foundation for subsequent extensions.

Theoretical Background and Related Work

Phase transformations in multi-component alloys

Phase transformations are fundamental processes governing microstructural evolution in metallic alloys and, by extension, determining critical properties such as strength, ductility, fracture toughness, thermal stability, and resistance to environmental degradation. In conventional alloy systems, transformation behavior is often tractable through relatively low-dimensional phase diagrams and well-characterized transformation mechanisms. However, in multi-component alloys, including high-entropy and medium-entropy alloys, phase transformations become substantially more complex due to the simultaneous presence of multiple principal elements. This compositional complexity dramatically increases the number of possible phases, metastable states, and transformation pathways, rendering intuitive or purely empirical prediction increasingly unreliable [11].

Transformations in multi-component alloys can broadly be categorized into solid-state transformations, including diffusionless (e.g., martensitic) and diffusion-controlled processes. These transformations are governed by an interplay between thermodynamic driving forces, which favor phase stability, and kinetic barriers, which control the rate and sequence of phase evolution. Unlike simpler alloys, where dominant mechanisms are clearly identifiable, multi-component systems often exhibit competing transformation routes, sluggish diffusion, and prolonged metastability, all of which complicate predictive modeling.

From a thermodynamic perspective, phase stability is determined by the minimization of Gibbs free energy, and equilibrium is defined by the condition in which the chemical potentials of all components are equal across coexisting phases. The Gibbs phase rule constrains the degrees of freedom in a system, but its practical application becomes increasingly abstract as the number of components rises [12]. In high-dimensional composition–temperature–pressure spaces, traditional phase diagrams lose their visual and analytical utility, necessitating alternative representations or surrogate modeling strategies.

Kinetic considerations further compound these challenges. Diffusion rates vary widely among constituent elements, and local compositional fluctuations can lead to heterogeneous nucleation behavior. As a result, transformations frequently deviate from equilibrium predictions, particularly under realistic processing conditions such as rapid cooling or non-isothermal treatments. Consequently, a comprehensive understanding of phase transformation pathways in multi-component alloys requires models that capture both equilibrium tendencies and non-equilibrium kinetics within a unified framework.

Recent literature underscores these challenges, emphasizing that elemental interactions—rather than individual elemental properties—play a decisive role in governing phase stability and transformation behavior in high-entropy systems [13, 14]. These studies highlight the inadequacy of extrapolating from lower-order alloy systems and point toward the need for new modeling paradigms capable of navigating complex, high-dimensional phase spaces.

Neural networks in materials modeling

The increasing availability of computational resources and materials databases has accelerated the adoption of neural networks in materials science, particularly for property prediction, materials screening, and inverse design. Feedforward neural networks, convolutional neural networks, and ensemble learning approaches have demonstrated strong performance in capturing non-linear relationships between alloy composition, processing parameters, and macroscopic properties [15]. These models are especially attractive for multi-component systems, where traditional analytical models struggle with combinatorial complexity.

In the context of phase-related predictions, machine learning models have been employed to classify phase stability, predict dominant phases, and estimate transformation-related properties. Common approaches rely on carefully selected descriptors—such as atomic size mismatch, electronegativity differences, and valence electron concentration—to encode

compositional information [16]. While such descriptor-based models have yielded valuable insights, their predictive scope is often limited to interpolation within the training domain.

A critical limitation of conventional neural networks in phase transformation modeling lies in their extrapolation behavior. Because these models are fundamentally statistical, they tend to perform poorly when queried outside the compositional or thermodynamic regimes represented in the training data. This issue is particularly acute in multi-component alloys, where experimental data are sparse and unevenly distributed across the design space. Moreover, unconstrained neural networks may generate predictions that violate known physical principles, such as predicting unstable phases as equilibrium states or neglecting kinetic limitations altogether.

These shortcomings highlight a fundamental tension in data-driven materials modeling: while neural networks excel at learning complex correlations, they lack an inherent understanding of causality or physical law. This limitation has driven growing interest in hybrid approaches that seek to retain neural networks' expressive power while embedding domain knowledge directly into the learning process.

Physics-constrained and physics-informed learning

Physics-constrained learning represents a methodological shift in machine learning, integrating governing physical laws into data-driven models to improve robustness, accuracy, and interpretability. A prominent embodiment of this philosophy is the development of physics-informed neural networks (PINNs), which incorporate partial differential equations, conservation laws, or constitutive relationships directly into the loss function [17, 18]. By penalizing violations of known physics during training, PINNs ensure that learned solutions remain physically admissible, even when data are limited.

In materials science, PINNs have been successfully applied to inverse problems, surrogate modeling, and property prediction, particularly in scenarios with scarce or noisy data [19, 20]. These studies demonstrate that embedding physics into the learning process can significantly enhance generalizability and reduce overfitting, effectively serving as physics-based regularization.

Despite these advances, existing PINN applications in materials science have focused mainly on field-variable prediction—such as stress, strain, or temperature evolution—rather than on discrete, path-dependent phenomena, such as phase transformation sequences. Moreover, many implementations assume a predefined governing equation, which may be challenging to specify uniquely for complex multi-component phase transformations involving coupled thermodynamic and kinetic effects.

This limitation suggests the need for a more flexible interpretation of physics-constrained learning—one that moves beyond strict PDE enforcement and instead integrates higher-level physical principles, such as energy minimization and diffusion constraints, into neural network training. Such an approach would be particularly well-suited for modeling phase transformation pathways, where the objective is not merely to solve equations, but to predict physically consistent sequences of phase evolution.

Synthesis of literature

Collectively, the literature reveals a clear trend toward hybrid modeling strategies that combine machine learning with physical insight to overcome the limitations of purely data-driven or purely physics-based approaches [21–28]. In materials science, this convergence reflects a growing recognition that complex systems—such as multi-component alloys—cannot be adequately described by either paradigm in isolation.

While significant progress has been made in applying machine learning to phase stability prediction and in developing physics-informed neural networks for materials problems, a notable gap remains in addressing phase transformation pathways in multi-component alloys. Existing studies tend to focus on equilibrium phase classification, property

prediction, or isolated physical processes, rather than on the integrated, time-dependent evolution of phases under realistic conditions.

This gap motivates the development of a novel conceptual framework that explicitly targets transformation pathways while embedding thermodynamic and kinetic constraints within a neural network architecture. By synthesizing insights from phase transformation theory, neural network modeling, and physics-constrained learning, the proposed framework seeks to advance theoretical understanding and provide a foundation for future computational and experimental investigations.

Conceptual framework: Physics-constrained neural networks

Conceptual overview of PCNNs

The proposed framework introduces physics-constrained neural networks (PCNNs) as a theoretical modeling paradigm for predicting phase transformation pathways in multi-component alloys. The central objective of the framework is to couple the representational flexibility of neural networks with the rigor of thermodynamic and kinetic principles, enabling physically consistent predictions across high-dimensional compositional and processing spaces.

At its core, the PCNN framework accepts alloy composition, temperature, and time as input variables, reflecting the primary state parameters governing phase evolution. These inputs are mapped through a deep neural network to outputs describing the sequence of phase transformations, associated stability regions, and transformation kinetics. Unlike conventional data-driven models, the PCNN does not rely solely on statistical fitting; instead, it embeds domain knowledge directly into the learning objective.

The architecture follows a standard feedforward neural network topology: an input layer, multiple hidden layers, and an output layer. The defining novelty of the framework lies not in the network topology itself, but in the formulation of the loss function, which explicitly incorporates physics-based constraints. Thermodynamic consistency is enforced through constraints derived from Gibbs free energy minimization, ensuring that predicted phase states satisfy stability criteria. In parallel, kinetic constraints, informed by diffusion theory, regulate time-dependent behavior by penalizing violations of mass transport relations.

Embedding physical principles as constraints

These constraints act as regularization terms, guiding the optimization process toward solutions that are not only accurate but also physically admissible. The integration of thermodynamic and kinetic laws into the optimization objective necessitates a precise mapping of the physical principles to their influence on model behavior, as shown in [Table 2](#).

Table 2. Physical principles incorporated into the physics-constrained neural network (PCNN) framework and their functional role in enforcing physically consistent predictions

Physical domain	Governing principle	Conceptual mathematical form	Role in loss function	Effect on predictions
Thermodynamics	Gibbs free energy minimization	$\Delta G \rightarrow \text{minimum}$	Penalizes unstable phase states	Ensures phase stability
Phase equilibria	Gibbs phase rule	DOF constraints	Limits the unphysical phase coexistence	Reduces spurious phases
Kinetics	Diffusion-controlled transformation	$J = -D\nabla C$	Enforces time-dependent behavior	Captures non-equilibrium pathways
Mass conservation	Continuity constraints	$\partial C/\partial t$ balance	Penalizes mass imbalance	Maintains physical realism

By embedding physical principles directly into the training objective, the PCNN framework effectively balances data fidelity and physical realism. This approach is particularly advantageous in multi-component alloy systems, where experimental data are sparse, and equilibrium assumptions alone are insufficient to describe observed transformation behavior. The constrained learning strategy enables the model to explore complex transformation pathways while maintaining adherence to fundamental laws, reducing the likelihood of unphysical predictions that often arise in unconstrained neural networks.

The overall conceptual architecture of the proposed PCNN framework is depicted in **Figure 1**, illustrating how compositional and processing inputs are propagated through the network. At the same time, thermodynamic and kinetic constraints actively shape the learning process toward physically consistent phase-transformation predictions.

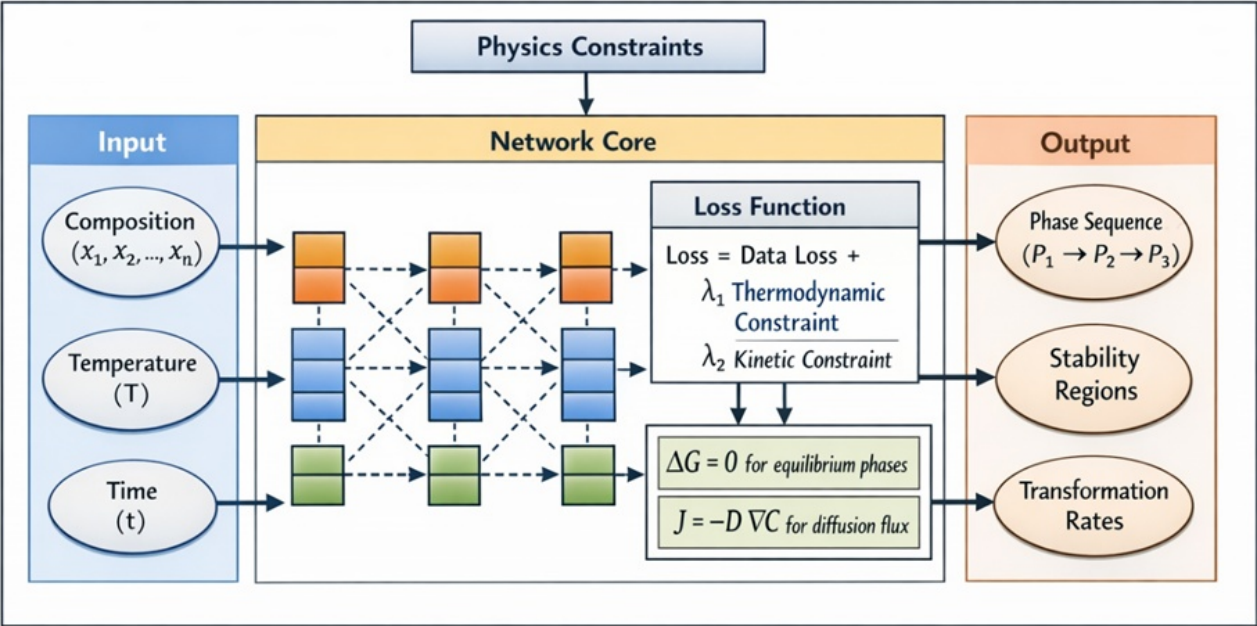


Figure 1. Conceptual architecture of the physics-constrained neural network (PCNN) framework for modeling phase transformation pathways in multi-component alloys

Architecture as an epistemic system

The proposed framework provides a theoretically grounded foundation for modeling phase transformation pathways in multi-component alloys. By integrating physics into model optimization rather than post hoc correction, the PCNN paradigm offers a coherent, extensible approach to advancing AI-assisted materials design.

The effect of physics-based constraints on predicted phase-transformation trajectories is conceptually illustrated in **Figure 2**, contrasting PCNN-guided evolution along physically admissible pathways with the unconstrained trajectories produced by purely data-driven models.

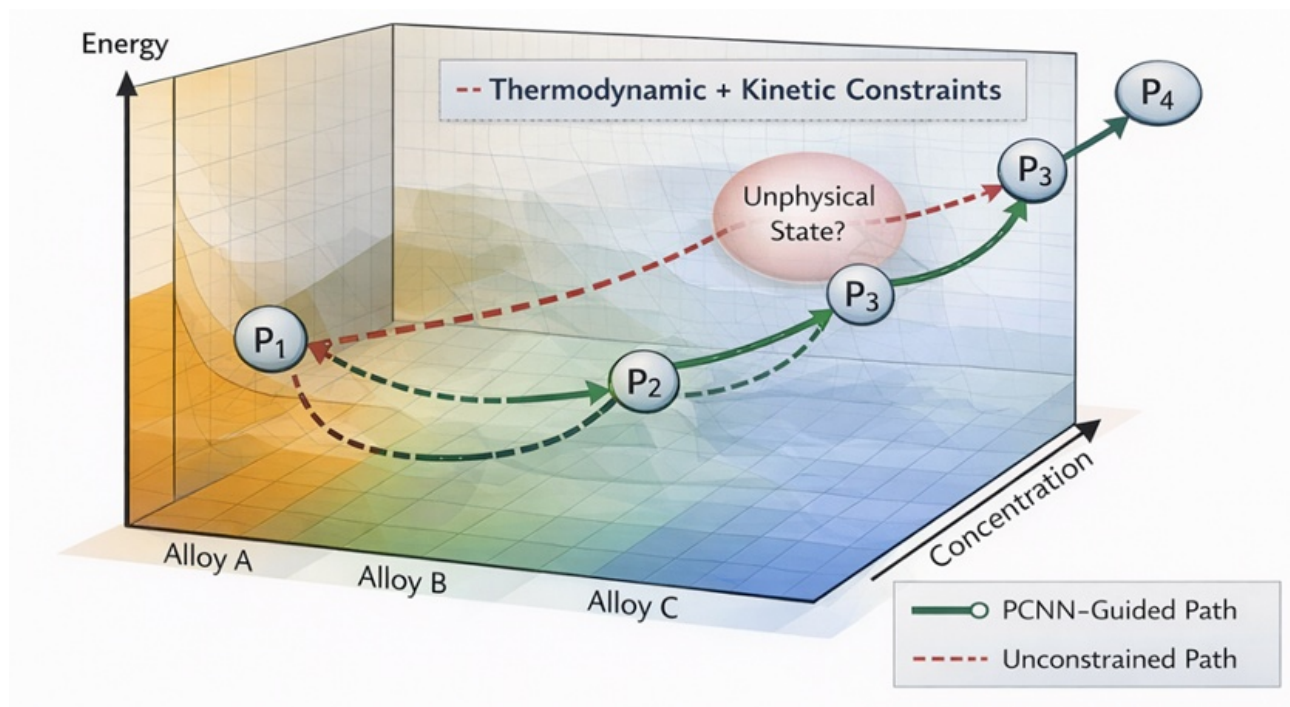


Figure 2. A conceptual visualization of phase-transformation pathways in a multi-component

The three-dimensional phase space, spanned by composition and energy coordinates, illustrates how thermodynamic and kinetic constraints restrict the model to physically admissible trajectories. The solid green pathway represents the PCNN-guided evolution through successive phases ($P_1 \rightarrow P_2 \rightarrow P_3 \rightarrow P_4$), remaining within energetically and kinetically feasible regions of the phase landscape. In contrast, the dashed red trajectory illustrates the behavior of an unconstrained machine-learning model, which may traverse energetically unfavorable or unphysical areas of phase space. The highlighted “unphysical state” region emphasizes the risk of violating fundamental physical laws when constraints are not enforced. Overall, the figure demonstrates that embedding thermodynamic and kinetic principles into the learning framework guides predictions toward realistic transformation pathways, thereby improving physical consistency and interpretability in alloy phase modeling.

This framework ensures predictions are physically consistent, offering a new tool for materials design.

Propositions

The proposed physics-constrained neural network (PCNN) framework offers a theoretical basis for advancing predictions of phase transformation pathways in multi-component alloys. Drawing from the synthesis of recent literature, several propositions can be derived to articulate the expected theoretical advantages and implications of this approach. These propositions are grounded in integrating physical principles into neural network structures, aiming to bridge gaps in current modeling paradigms.

Proposition 1: Incorporating thermodynamic constraints, such as Gibbs free energy minimization, into the loss function of PCNNs will enhance the model’s ability to predict equilibrium phase sequences in multi-component alloys by ensuring compliance with fundamental stability criteria. This proposition stems from the observation that traditional neural networks often fail to incorporate energy-based rules, leading to predictions that deviate from physical reality [1, 2]. By embedding these constraints, the framework theoretically reduces the risk of unphysical outputs, particularly in systems with high compositional complexity where phase stability is sensitive to element interactions.

Proposition 2: Kinetic constraints, derived from diffusion equations, when integrated into PCNN architectures, will improve the prediction of non-equilibrium transformation pathways by accounting for time-dependent processes in alloy systems. The literature indicates that kinetic factors are often underrepresented in data-driven models, yet they are essential for capturing diffusion-controlled transformations [3, 4]. This proposition posits that such constraints will, in theory, allow the model to simulate pathway sequences under varying cooling rates, offering a more comprehensive view than static thermodynamic models.

Proposition 3: PCNNs will exhibit superior interpretability compared to black-box neural networks, owing to their explicit physical constraints, enabling the extraction of meaningful insights into phase transformation mechanisms. The opacity of conventional machine learning models limits their utility in scientific inquiry [5, 6]. Theoretically, the constrained structure facilitates back-propagation analysis to identify how physical laws influence predictions, thereby aiding understanding of element-specific contributions to phase behavior.

Proposition 4: In sparse data regimes characteristic of multi-component alloys, PCNNs will demonstrate improved generalizability through the regularization effect of physics constraints, reducing overfitting and enhancing extrapolation capabilities. Studies highlight the challenges of data scarcity in alloy design [7, 8]. This proposition suggests that by prioritizing physical consistency over data fitting alone, the framework can, in theory, extend predictions to unexplored compositional spaces.

Proposition 5: The modular design of PCNNs, allowing for the addition of alloy-specific constraints, will facilitate adaptability to diverse multi-component systems, promoting a unified theoretical approach across alloy classes. Existing models often require redesign for different systems [9, 10]. Theoretically, this modularity supports the framework’s application to high-entropy alloys and beyond, fostering broader theoretical advancements in materials science.

These propositions collectively underscore the potential of PCNNs to transform theoretical modeling in materials science, emphasizing rigor and physical fidelity.

Results and Discussion

The conceptual framework of physics-constrained neural networks (PCNNs) for predicting phase transformation pathways in multi-component alloys represents a significant theoretical advancement at the intersection of artificial intelligence and materials science. By embedding physical laws directly into the network’s architecture, the approach addresses key limitations of both traditional physics-based models and data-driven machine learning techniques. Conventional methods, such as CALPHAD, provide robust thermodynamic insights but struggle with kinetic complexities and computational scalability in high-dimensional compositional spaces [11, 12]. Conversely, pure neural networks excel in pattern recognition but may generate implausible results due to a lack of physical grounding [13, 14]. The PCNN framework theoretically mitigates these issues by enforcing constraints that align predictions with established principles, potentially enabling more reliable theoretical exploration of alloy behavior. The manner in which the physics-constrained neural network framework conceptually addresses key challenges in phase-transformation modeling is summarized in

Table 3.

Table 3. Theoretical advantages of the PCNN framework in addressing key challenges associated with phase transformation modeling in multi-component alloys

Alloy design challenge	Limitations of existing methods	PCNN advantage	Theoretical outcome
High-dimensional composition space	Combinatorial explosion	Physics-guided regularization	Efficient exploration

Sparse experimental data	Overfitting in ML	Constraint-driven learning	Improved generalizability
Non-equilibrium processing	Equilibrium bias	Kinetic constraints	Realistic pathways
Lack of interpretability	Black-box predictions	Explicit physical embedding	Mechanistic insight

One theoretical implication is the enhancement of predictive efficiency in materials design. Multi-component alloys, including high-entropy variants, offer expansive design opportunities, but navigating their phase spaces requires tools that balance accuracy and computational cost [15, 16]. PCNNs, through their constrained optimization, could theoretically accelerate the identification of stable phases and transformation routes, facilitating rapid theoretical screening for applications in extreme environments. Furthermore, the framework’s emphasis on interpretability aligns with the need for mechanistic understanding in theoretical studies, allowing researchers to dissect how constraints influence outcomes [17, 18].

However, conceptual limitations must be acknowledged. The framework assumes that selected physical constraints comprehensively capture relevant phenomena, yet in complex alloys, overlooked interactions—such as magnetic effects or defect influences—could theoretically compromise accuracy [19, 20]. Additionally, the weighting of constraints in the loss function introduces theoretical trade-offs between physical adherence and model flexibility, potentially requiring optimization strategies that are not yet fully defined [21, 22]. These aspects highlight the need for further theoretical refinement to ensure robustness across diverse alloy systems.

Future theoretical developments could extend the framework by incorporating multiscale constraints and linking atomic-level kinetics with macroscopic properties [23, 24]. Such integrations might enable holistic modeling of alloy performance, advancing theoretical paradigms in applied artificial intelligence for materials science.

Conclusion

This manuscript has developed a novel conceptual framework for physics-constrained neural networks tailored to predict phase transformation pathways in multi-component alloys. By integrating thermodynamic and kinetic principles into the neural architecture, the approach ensures physically consistent predictions and addresses gaps in existing models. The propositions outline theoretical benefits in terms of accuracy, interpretability, and generalizability, while the discussion explores their implications and limitations. Ultimately, this framework contributes to the theoretical foundation of AI-driven materials science and has the potential to inform future alloy design strategies.

Acknowledgements

None

Conflict of interest

None

Financial support

None

Ethics statement

None

Received: 21 Feb 2023

Revised: 25 Apr 2023

Accepted: 22 May 2023

Published online: 18 July 2023

Rights and permissions

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

- Zhang E, Dao M, Karniadakis GE, Suresh S. Analyses of internal structures and defects in materials using physics-informed neural networks. *Sci Adv.* 2022;8(7):eabk0644.
- Rathod VT, Ramuhalli P. Physics-informed neural networks for identification of material properties using standing waves. Oak Ridge National Laboratory Report. 2021.
- Yan CA, Vescovini R, Dozio L. A framework based on physics-informed neural networks and extreme learning for the analysis of composite structures. *Comput Struct.* 2022;265:106761.
- Zhong X, Gallagher B, Liu S, Kailkhura B, Hiszpanski A, Han TY. Explainable machine learning in materials science. *npj Comput Mater.* 2022;8:204.
- Shukla K, Jagtap AD, Blackshire JL, Sparkman D, Karniadakis GE. A physics-informed neural network for quantifying the microstructure properties of polycrystalline Nickel using ultrasound data. *IEEE Signal Process Mag.* 2021;38(6):98-107.
- Sharma S, Awasthi R, Sastry YS, Budarapu PR. Physics-informed neural networks for estimating stress transfer mechanics in single lap joints. *J Zhejiang Univ Sci A.* 2021;22(8):621-31.
- Haghighat E, Raissi M, Moure A, Gomez H, Juanes R. A physics-informed deep learning framework for inversion and surrogate modeling in solid mechanics. *Comput Methods Appl Mech Engrg.* 2021;379:113741.
- Akhare D, Luo T, Wang J-X. Physics-integrated Neural Differentiable (PiNDiff) Model for Composites Manufacturing. *ChemRxiv.* 2022.
- Lee K, Ayyasamy MV, Delsa P, Hartnett TQ, Balachandran PV. Phase classification of multi-principal element alloys via interpretable machine learning. *npj Comput Mater.* 2022;8:25.
- Beniwal D, Singh P, Gupta S, Kramer MJ, Johnson DD, Ray PK. Distilling physical origins of hardness in multi-principal element alloys directly from ensemble neural network models. *npj Comput Mater.* 2022;8:153.
- Yang Y, Zhao L, Zong HX. Taking materials dynamics to new extremes using machine learning interatomic potentials. *J Mater Inf.* 2021;1:10.

Subedi U, Poudel S, Gyanwali K, Amorim Coutinho Y, Matula G, Kunwar A. State-of-the-Art Review on the Aspects of Martensitic Alloys Studied via Machine Learning. *Metals*. 2022;12(11):1884.

Si SP, Fan BJ, Liu XW, Zhou T, He C, Song DD, et al. Study on strengthening effects of Zr-Ti-Nb-O alloys via high throughput powder metallurgy and data-driven machine learning. *Mater Des*. 2021;206:109777.

Arróyave R. Phase stability through machine learning. *J Phase Equilib Diffus*. 2022;43:606-28.

Li R, Xie L, Wang WY, Liaw PK, Zhang Y. High-Throughput calculations for high-entropy alloys: A brief review. *Front Mater*. 2020;7:290.

Frydrych K, Karimi K, Pecelerowicz M, Alvarez R, Dominguez-Gutiérrez FJ, Rovaris F, et al. Materials informatics for mechanical deformation: A review of applications and challenges. *Materials (Basel)*. 2021;14(19):5764.

Da Costa Garcia Filho F, Ritchie RO, Meyers MA, Monteiro SN. Cantor-derived medium-entropy alloys: bridging the gap between traditional metallic and high-entropy alloys. *J Mater Res Technol*. 2022;17:1868-95.

Dobrzański LA. Advanced Composites with Aluminum Alloys Matrix and Their Fabrication Processes. In: Dobrzański LA, editor. *Advanced Aluminium Composites and Alloys*. London: IntechOpen; 2021. Available from: <https://www.intechopen.com/chapters/77648>.

Liu D, Wang Y. Metal additive manufacturing process design based on physics constrained neural networks and multi-objective Bayesian optimization. *Manuf Lett*. 2022;33(Suppl):817-27.

Xu K, Huang DZ, Darve E. Learning Constitutive Relations using Symmetric Positive Definite Neural Networks. *J Comput Phys*. 2021;426:109943.

Taverniers S, Hall EJ, Katsoulakis MA, Tartakovsky DM. Mutual information for explainable deep learning of multiscale systems. *J Comput Phys*. 2021;444:110551.

Peng J, Yamamoto Y, Hawk JA, Lara-Curzio E, Shin D. Coupling physics in machine learning to predict properties of high-temperatures alloys. *Npj Comput Mater*. 2020;6:141.

Treherm W, Ortiz-Ayala R, Atli KC, Arroyave R, Karaman I. Data-driven shape memory alloy discovery using Artificial Intelligence Materials Selection (AIMS) framework. *Acta Mater*. 2022;228:117751.

Rao Z, Tung PY, Xie R, Wei Y, Zhang H, Ferrari A, et al. Machine learning-enabled high-entropy alloy discovery. *Science*. 2022;378(6615):78-85.

Fu H, Zhang H, Wang C, Yong W, Xie J. Recent progress in the machine learning-assisted rational design of alloys. *Int J Miner Metall Mater*. 2022;29(4):635-44.

Yang Y, Zhao L, Han CX, Ding XD, Lookman T, Sun J, et al. Taking materials dynamics to new extremes using machine learning interatomic potentials. *J Mater Inf*. 2021;1:10.

Hmede R, Chapelle F, Lapusta Y. Review of neural network modeling of shape memory alloys. *Sensors (Basel)*. 2022;22(15):5610.

Liyanage M, Reith D, Eyert V, Curtin WA. Machine learning for metallurgy V: A neural-network potential for zirconium. *Phys Rev Mater*. 2022;6(6):063804.