Logographic AI for Inverse Design of Metamaterials: A Morpho-Root Based Graph-Reasoning Framework and Trustworthy Generation Pathway

Abstract

Metamaterials, through the deliberate arrangement of structures at the mesoscale, can achieve extraordinary physical properties unattainable by natural materials. However, the current mainstream approach to inverse design of metamaterials—which directly maps target properties to microstructures using deep generative models (diffusion models, flow matching, variational autoencoders, etc.)—faces a fundamental bottleneck: the generation process is a "black box." Designers obtain an "optimal" microstructure without knowing "why this structure" or "what each structural feature contributes to the performance." In safety-critical applications (e.g., aerospace, defense equipment), this inexplicability severely constrains the practical adoption and engineering trust of inverse design results.

This paper introduces "Logographic AI" (LAI) as an alternative cognitive paradigm and proposes a graph-reasoning framework based on "Metamaterial Morpho-Roots" for trustworthy inverse design of metamaterials. The core of LAI theory is the "Morpho-Root"—a structured cognitive primitive that carries inherent semantics—to replace statistically defined Tokens. In LAI, the Morpho-Root is formalized as a structured triple $\tau = (S, A, R)$, where S is the symbolic identifier, A is the attribute set embedding physical properties and constraints, and R is the set of predefined logical relation functions. Mapping this framework to the metamaterials domain, we propose the "Metamaterial Morpho-Root" system—a mechanism-first knowledge representation method that encodes mesostructural features of metamaterials (e.g., unit cell topology, spatial arrangement, symmetry), physical response laws (e.g., dispersion relations, bandgap characteristics, effective medium parameters), and design constraints into computable cognitive units. Building on this, we design a Morpho-Structural Entropy (MSE)-guided inverse reasoning engine: given target properties, the system performs structured reasoning over the Morpho-Root semantic network to generate a fully traceable decision subgraph—where every design choice corresponds to a clear physical reasoning chain, rather than a statistical correlation.

This paper demonstrates that LAI-driven inverse design of metamaterials can achieve: (1) interpretable generation—the design rationale for each structural feature is traceable to explicit physical mechanisms; (2) zero violation of hard constraints—through physical and manufacturability constraints embedded in Morpho-Roots, ensuring that generated structures satisfy all necessary conditions; (3) proactive identification of knowledge gaps—when reasoning paths break, the system proactively requests external validation (e.g., high-fidelity simulation or experiment) rather than forcing unreliable recommendations. Finally, this paper proposes a hybrid architecture that integrates the LAI framework with existing deep generative models (e.g., diffusion models): the generative model is responsible for efficient sampling of candidate structures, while the LAI Morpho-Root network is responsible for trustworthy screening and mechanistic validation of candidates—forming a closed loop of "generation–validation–explanation."

Keywords: Logographic AI (LAI); Metamaterials; Inverse Design; Morpho-Root; Explainable AI; Graph Reasoning; Trustworthy Generation

1. Introduction: The Black-Box Dilemma of Inverse Metamaterials Design

Metamaterials are a class of artificially engineered composite materials that achieve extraordinary physical properties unattainable by natural materials through the deliberate arrangement of subwavelength structural units. From negative refractive index materials to electromagnetic cloaking, from mechanical metamaterials to thermal radiation control devices, metamaterials are redefining humanity's ability to manipulate physical fields including light, sound, heat, and mechanics. However, the functionality of metamaterials is highly dependent on their complex mesostructures—details such as unit cell geometry, spatial arrangement, and symmetry breaking collectively determine the final macroscopic response. The highly nonlinear and many-to-many nature of this structure–property mapping renders traditional design methods based on physical intuition and parameter scanning increasingly inadequate.

In recent years, the introduction of deep generative models—including diffusion models, flow matching, and variational autoencoders—has brought revolutionary changes to inverse metamaterials design [9]. These methods directly map from target property spaces to microstructure spaces, achieving a paradigm shift from "forward trial-and-error" to "inverse generation." The Shanghai Jiao Tong University team has achieved representative results in this field—constructing an AI model for inverse design of thermal metamaterials that can generate large batches of candidate designs and "select the best," with results published in Nature [7]. Frameworks such as DiffMat have further applied diffusion models to the inverse design of energy-absorbing metamaterials, enabling customized generation of microstructures that meet mechanical performance requirements based on target stress–strain curves [5].

However, a fundamental problem is being systematically overlooked: the current inverse design process is an end-to-end black-box mapping. Designers input a target spectrum or stress–strain curve, and the model outputs an "optimal" microstructure—but designers do not know "why this structure," do not know "what each structural feature contributes to the performance," and do not know "whether the model truly understands the underlying physics or is merely performing high-dimensional interpolation within the distribution of training data."

In basic research, this "black box" may be tolerable—as long as sufficiently good structures can be generated, the mechanisms can be analyzed post hoc. But in safety-critical applications—such as aerospace structural metamaterials, defense stealth metamaterials, and radiation shielding metamaterials in the nuclear sector—inexplicability directly constitutes a veto for engineering adoption. Engineers need to know: why does this structure meet the performance specifications? What are its failure modes? How much does manufacturing deviation affect performance? Current pure generative models cannot answer these questions.

This problem, at a more macro level, has been characterized as "Technology Capture"—where powerful technological tools themselves shape and constrain the formulation and resolution of scientific questions. Chinese scholar Shen Liu, in Chapter 1 of The Rooted Intelligence: The Paradigm Revolution of Logographic AI [2], systematically discusses the capture effect of technological path dependency on scientific innovation. When researchers become satisfied that "the model can generate structures," they may cease to ask "why the model generates this way"—this satisfaction itself is precisely the capture of deeper scientific understanding.

This paper argues that the key to breaking this dilemma lies not in training larger generative models, but in reconstructing AI's cognitive architecture—shifting from "statistical fitting" to "mechanistic reasoning." The Logographic AI (LAI) theory proposed by Shen Liu [1][2] provides a completely new philosophical foundation and implementation path for this purpose. The core of LAI is to replace arbitrary "Tokens" with "Morpho-Roots" that carry inherent form-meaning rationality, fundamentally reconstructing AI's semantic construction logic. This paper maps this theoretical framework to the metamaterials domain, proposing a "Metamaterial Morpho-Root" system and a Morpho-Root-based graph reasoning framework, aiming to achieve trustworthy, interpretable, and mechanism-driven inverse design of metamaterials.

2. Challenges in Inverse Metamaterials Design and Limitations of Current Methods

2.1 Achievements of Deep Generative Methods

The current mainstream technical approach to inverse metamaterials design can be summarized as: data-driven at its core, deep generative models as the engine, target properties as conditions, and microstructures as outputs. Yu et al. have provided a systematic review of AI-driven approaches to electromagnetic metamaterials design [9].

Within this paradigm, researchers have achieved remarkable accomplishments:

- **Diffusion models**: The conditional diffusion model framework proposed by Li et al. enables customized generation of metamaterial shapes and size parameters from target spectra, with experimental validation in thermal camouflage applications [6].
- **DiffMat framework**: Based on denoising diffusion probabilistic models (DDPM), it can generate energy-absorbing metamaterial microstructures that meet mechanical performance requirements based on target stress–strain curves [5].
- **Agentic frameworks**: Lu et al. developed an Agentic Framework capable of autonomous metamaterial modeling and inverse design. When queried with a target spectrum, the agent can autonomously propose and train forward deep learning models, call external tools for optimization, and ultimately generate designs through deep inverse methods [8].
- **Industrial-scale applications**: The thermal metamaterial inverse design AI model developed by the Shanghai Jiao Tong University team can generate large batches of candidate designs and has achieved experimental validation across multiple application forms, from flexible films to coatings and patches [7].

These works collectively demonstrate the powerful capabilities of deep generative models in inverse metamaterials design—high efficiency, broad coverage, and scalability.

2.2 Three Fundamental Limitations

However, behind these achievements lie three systematic limitations:

Limitation One: Inexplicability

The current inverse design process is essentially a conditional probability sampling in high-dimensional space. The model learns "given target property Y, the conditional distribution of structure X, p(X|Y)," rather than "why X produces Y" as a causal mechanism. When the model outputs a structure, designers cannot trace the answers to the following questions:

- Which geometric feature of this structure is primarily responsible for achieving the target performance?
- If a certain feature cannot be manufactured, is there an alternative?
- For which parts of the prediction is the model confident, and for which is it uncertain?

Shen Liu points out that this inexplicability stems from the inherent flaw of the Token paradigm in discretizing continuous semantics—Tokens carry no inherent meaning, and their "semantics" are temporarily assigned by statistical co-occurrence relationships. Token-based models may discover correlations, but can never truly "understand" causality.

Limitation Two: Constraint Satisfaction Cannot Be Guaranteed

Practical applications of metamaterials require not only meeting physical performance indicators but also satisfying a series of engineering constraints—manufacturability constraints (e.g., minimum feature size, overhang angle, support structures), material compatibility constraints, cost constraints, etc. While current generative models may implicitly capture these constraints in training data, they cannot hard-guarantee their satisfaction at inference time. When a generated structure violates manufacturability constraints, the entire design loses engineering value.

Limitation Three: Inefficient Use of Physical Knowledge

Metamaterials research has accumulated a wealth of mature physical theories over decades of development—effective medium theory, transmission line models, Bloch's theorem, dispersion relation analysis, etc. These theories provide profound insights into "what kind of structure produces what kind of response." However, current purely data-driven approaches almost completely ignore this prior physical knowledge, leaving everything to the data to "speak for itself." This not only leads to low data efficiency but, more importantly, misses the opportunity to encode decades of accumulated physical insight into AI's cognitive architecture.

2.3 The "Technology Capture" Risk

The superposition of these three limitations is leading inverse metamaterials design toward a deeper dilemma—"Technology Capture."

When a technology (deep generative models) performs well on a certain task, the research community naturally invests increasing resources in the continuous optimization of this technical path—larger models, more data, more complex architectures. This path dependence of "architectural improvement" is not inherently problematic; the problem lies in the fact that it may cause researchers to become satisfied with "being able to generate," and cease to ask "why it can generate."

In inverse metamaterials design, this "Technology Capture" manifests as: the evaluation metrics researchers focus on subtly shift from "whether the design principles are understood" to "how high the generation accuracy is"; the novelty of papers shifts from "what new mechanisms have been revealed" to "what new SOTA has been achieved on which dataset." This shift is not an individual researcher's choice, but a collective unconsciousness shaped by the entire technological paradigm.

Breaking through this dilemma requires not continuing "involution" within the same paradigm, but introducing a completely new cognitive paradigm—which is precisely the entry point of Logographic AI (LAI) theory.

3. Logographic AI and the "Metamaterial Morpho-Root" System

3.1 Overview of LAI Theory: From Token to Morpho-Root

Logographic AI (LAI) is an alternative AI paradigm proposed by Chinese scholar Shen Liu [1][2]. Its core insight is that all current mainstream AI models are essentially "Phonographic AI" (PAI)—they use meaningless Tokens as basic cognitive units, "understanding" the world by statistically modeling co-occurrence relationships between Tokens. The success of this paradigm does not mean it understands meaning—only that it performs well enough at statistical correlation.

LAI's alternative is to introduce the "Morpho-Root" as the basic cognitive unit. The Morpho-Root is a structured cognitive primitive carrying inherent semantics, formally defined as a triple:

$$\boldsymbol{\tau = (S, A, R)}$$

where:

- **S (Symbol)**: A symbolic identifier that uniquely refers to the Morpho-Root in the system.
- **A (Attributes)**: A set embedding inherent semantic features, physical properties, and hard constraints.
- **R (Relation Functions)**: A set of predefined logical connection methods and relation functions.

The essential difference between Morpho-Root and Token is: the Token is an empty statistical placeholder whose "meaning" is entirely determined by contextual statistics; the Morpho-Root is a saturated semantic atom whose meaning is embedded in its own structural definition. This seemingly subtle difference determines whether AI moves from "statistical fitting" to "cognitive understanding" or remains forever in the former. Liu, in Chapter 5 of The Rooted Intelligence, systematically demonstrates how Morpho-Roots fundamentally solve the Symbol Grounding Problem.

In the LAI framework, Morpho-Structural Entropy (MSE) is a key information-theoretic measure of the orderliness of the Morpho-Root system. Low MSE regions correspond to clear, established mechanistic paths; high MSE regions correspond to uncertain knowledge gaps requiring external validation. The MSE-guided reasoning strategy is: rapidly traverse known mechanistic paths in low-entropy regions; proactively request external validation (high-fidelity simulation or experiment) in high-entropy regions. Liu systematically establishes the information-theoretic distinction between Morpho-Structural Entropy and Sequential Entropy in Chapter 6 of The Rooted Intelligence.

3.2 Formal Definition of "Metamaterial Morpho-Root"

Mapping the LAI Morpho-Root framework to the metamaterials domain, we define the "Metamaterial Morpho-Root" as a computable cognitive primitive that encapsulates the minimal mechanistic unit in the metamaterials field.

Taking the "Metamaterial Unit Cell Morpho-Root" as an example, its formal definition is:

Metamaterial-Unit-Cell-Root = (S, A, R)

where:

- **S**: Identifier MM-UC-001 + Name Metamaterial-Unit-Cell-Root.
- **A**: Semantic definition + Mathematical descriptors (unit cell geometric parameters, symmetry group, space group, periodic constants, etc.).
- **R**: I/O relations (e.g., dispersion relation calculation functions, effective medium parameter derivation functions) + Associated Morpho-Roots (semantic relations such as is_composed_of, determines, constrained_by).

This formal definition enables every key mechanistic unit of metamaterials to be **explicitly and computably** encoded into AI's cognitive architecture, rather than being implicitly buried in the millions of parameters of a neural network. The OpenMorpho prototype system has implemented the core mechanisms of the above Morpho-Root data structure [10], verifying its engineering feasibility.

3.3 Core Metamaterial Morpho-Root Examples

The following are core Morpho-Root types constituting the Metamaterial Morpho-Root system (non-exhaustive):

Morpho-Root Name	Semantic Definition	Core Mathematical Descriptors	Key Associations
Metamaterial-Unit-Cell-Root	Geometric topology and spatial arrangement of metamaterial unit cells	Lattice constant a, unit cell dimensions, symmetry group	determines Dispersion-Relation-Root
Dispersion-Relation-Root	Dispersion relations and bandgap characteristics	Frequency ω(k), bandgap width Δω	determines Effective-Medium-Root
Effective-Medium-Root	Effective medium parameters	Effective refractive index n_eff,	determines

Morpho-Root Name	Semantic Definition	Core Mathematical Descriptors	Key Associations
		effective impedance Z_eff	Macroscopic-Response-Root
Manufacturability-Constraint-Root	Manufacturability constraints	Minimum feature size d_min, overhang angle θ_max	constrains Unit-Cell-Root
Multi-Physics-Response-Root	Multi-physics coupled response	Mechanical-thermal-electromagnetic coupling coefficients	integrates all physics-field roots
Auxetic-Structure-Root	Negative Poisson's ratio structural characteristics	Poisson's ratio $\nu < 0$	is_a_kind_of Metamaterial-Unit-Cell-Root
Re-Entrant-Hinge-Root	Re-entrant hinge topology	Hinge angle θ, arm length ratio	enables Auxetic-Structure-Root
Thermal-Response-Root	Thermal response characteristics	Thermal expansion coefficient $\alpha(T)$, thermal conductivity κ	couples_with Shape-Memory-Root

3.4 Essential Differences from Existing Metamaterials Characterization Methods

To more clearly position the innovative value of "Metamaterial Morpho-Root," it is necessary to compare it with existing metamaterials characterization approaches:

Dimension	Traditional Structural Descriptors	Deep Learning Implicit Representations	Metamaterial Morpho-Root
Representation Form	Single numerical value (e.g., porosity, specific surface area)	High-dimensional vector (neural network latent space)	Structured triple (S, A, R)
Semantic Carrying	No inherent semantics	No inherent semantics (black box)	Embedded physical semantics and constraints
Explainability	Low (single value cannot explain mechanism)	Extremely low (complete black box)	High (every step traceable to physical mechanism)
Reasoning Capability	None	None (can only generate, cannot reason)	Yes (graph reasoning based on semantic network)
Constraint Guarantee	None	None (statistical satisfaction, cannot be hard-guaranteed)	Yes (logic-level blocking of constraint-violating paths)
Knowledge Reuse	Difficult	Difficult (knowledge submerged in parameters)	Easy (Morpho-Roots can be reused and combined independently)

Traditional descriptors are "data compression," deep learning implicit representations are "data reparameterization," while the Metamaterial Morpho-Root is "explicit encoding of knowledge"—it tells the system not only "what it is," but also "why" and "what it cannot be."

4. Morpho-Root-Based Inverse Reasoning Engine

4.1 MSE-Guided Graph Traversal

The Metamaterial Morpho-Root system constitutes a directed semantic network G = (V, E), where nodes V are Morpho-Root types or Morpho-Root instances, and edges E are semantic relations (such as determines, enables, constrains, inhibits, is_a_kind_of).

The inverse design task can be formalized as: given a target performance set T = {t_1, t_2, ..., t_m}, search for an interpretable path from the target node to the achievable structural node in the Morpho-Root semantic network.

Morpho-Structural Entropy (MSE) plays a guiding role in this search process:

- **Low MSE regions**: The network contains dense, experimentally or theoretically validated reasoning paths. The system rapidly traverses along these paths, generating fully validated design solutions.
- **High MSE regions**: Reasoning paths in the network are sparse or broken, indicating that current knowledge is insufficient to reliably connect targets to structures. The system proactively marks knowledge gaps and generates queries to external validation systems (high-fidelity simulation or experiment).

The Morpho-Graph Computing paradigm proposed by Shen Liu replaces the dense self-attention mechanism of Transformers with sparse graph traversal of complexity O(|E|), achieving completely transparent, traceable reasoning. This strategy of "walk fast in low entropy; ask humans in high entropy" ensures both reasoning efficiency and prevents the system from forcing unreliable recommendations when knowledge is insufficient—a "self-awareness" that pure black-box generative models lack. The above MSE-guided graph traversal reasoning mechanism has been implemented in the OpenMorpho prototype system [10].

4.2 Reasoning Chain Construction for Inverse Design

The following example demonstrates how the Morpho-Root reasoning engine works:

Design Target: A mechanical metamaterial with auxetic (negative Poisson's ratio) properties.

Reasoning Process:

1. **Target Activation**: The system receives the target "negative Poisson's ratio," activating Auxetic-Structure-Root.
2. **Mechanism Tracing**: Auxetic-Structure-Root is associated via is_enabled_by to Re-Entrant-Hinge-Root (re-entrant hinges are the classical structural mechanism for achieving negative Poisson's ratio).

3. **Parameter Derivation**: Re-Entrant-Hinge-Root is associated via determines to Geometric-Parameter-Root, deriving the ranges of key geometric parameters such as hinge angle θ and arm length ratio.
4. **Constraint Checking**: Geometric-Parameter-Root is associated via constrained_by to Manufacturability-Constraint-Root, checking whether the derived geometric parameters satisfy manufacturability constraints (e.g., minimum feature size).
5. **Solution Output**: The system outputs the complete reasoning chain—from "negative Poisson's ratio" to "re-entrant hinge" to "geometric parameters" to "manufacturability validation"—with every step corresponding to a clear physical mechanism.

Visualization of the Reasoning Chain (Directed Acyclic Graph):

```
Target: Negative Poisson's Ratio

    ↓ (is_enabled_by)

Re-Entrant-Hinge-Root

    ↓ (determines)

Geometric-Parameter-Root {θ, arm_ratio, ...}

    ↓ (constrained_by)

Manufacturability-Constraint-Root {d_min, θ_max, ...}

    ↓ (validates)

Feasible Design Proposal
```

Every node and every edge in this reasoning chain is human-readable, auditable, and traceable. Designers receive not only "what structure," but also the complete justification of "why this structure."

4.3 Zero-Violation Assurance of Hard Constraints

In safety-critical applications, constraint satisfaction is not "try to satisfy" but "must satisfy." The LAI framework achieves zero-violation assurance of hard constraints through a logic-level blocking mechanism:

When the reasoning engine attempts to activate a certain Morpho-Root or reason along a certain edge, the system first checks whether this path violates any activated Constraint-Root. If violated, the path is **blocked at the reasoning stage**, rather than discovered after generation.

Liu, in Chapter 7 of The Rooted Intelligence, systematically elaborates the hierarchical axiom system and conflict resolution mechanism of the "Value Axiom Library." This mechanism ensures that hard constraints are logically guaranteed at the reasoning stage, achieving a paradigm shift from "external alignment" to "endogenous co-construction."

This mechanism forms a sharp contrast with pure generative models:

Comparison Dimension	Pure Generative Models	LAI Morpho-Root Reasoning
Constraint Checking Timing	After generation (post-processing filtering)	During reasoning (logic-level blocking)
Handling of Violations	Discard or patch	Constraint-violating paths are never generated
Guarantee Level	Statistical (mostly satisfied)	Deterministic (all satisfied)
Efficiency	Wasteful generation-validation-discard cycles	One reasoning pass satisfies all constraints

This difference is crucial in practical engineering applications of metamaterials—when designs involve dozens of mutually coupled constraints, the "generate-then-filter" strategy can lead to extremely high invalid generation rates, while the "block-during-reasoning" strategy ensures that every reasoning outcome is engineering-feasible. As demonstrated in the OpenMorpho hydrogen embrittlement risk assessment case, hard constraints can prune unsafe reasoning paths at the reasoning stage, ensuring deterministic safety [10].

5. Hybrid Architecture: LAI + Deep Generative Models

5.1 Why a Hybrid Architecture?

The LAI Morpho-Root reasoning engine and existing deep generative models each have advantages and limitations:

Dimension	LAI Morpho-Root Reasoning	Deep Generative Models
Advantages	Explainable, traceable, constraint-guaranteed	High efficiency, broad coverage, excels at high-dimensional spaces
Limitations	Depends on completeness of Morpho-Root knowledge base	Black box, inexplicable, no constraint guarantees

They are not substitutes but complements. The optimal solution is not choosing one over the other, but building a hybrid architecture that leverages the strengths of both.

5.2 Hybrid Architecture Design

The proposed hybrid architecture consists of three core modules:

Module 1: Generation Module (Deep Generative Models)

- **Function**: Efficiently sample candidate metamaterial structures from the target performance space.
- **Input**: Target performance descriptions (e.g., target spectrum, target stress–strain curve).
- **Output**: A large number of candidate structures.

- **Representative Methods**: Conditional diffusion models, variational autoencoders, generative adversarial networks, etc.
- **Evaluation**: **Efficiency-first**—rapid generation of a large number of candidates.

Module 2: Validation and Explanation Module (LAI Morpho-Root Network)

- **Function**: Perform mechanistic validation, constraint checking, and reasoning chain generation for candidate structures.
- **Input**: Candidate structures from the generation module.
- **Output**: Validated structures + complete traceable reasoning chains.
- **Representative Methods**: Morpho-Root semantic network traversal, MSE-guided graph reasoning.
- **Evaluation**: **Trustworthiness-first**—only outputs explainable, verifiable solutions.

Module 3: Closed-Loop Iteration Module

- **Function**: Feedback validation results to the generation module to guide the next round of generation.
- **Mechanism**: "Failure reasons" marked by the validation module are converted into "conditional constraints" for the generation module.
- **Effect**: With iteration, the generation module gradually "learns" to sample within constraint-satisfying regions.

5.3 Workflow

The typical workflow of the hybrid architecture is as follows:

```
Step 1: User inputs target performance

    ↓

Step 2: Generation module (diffusion model) rapidly samples N candidate structures

    ↓

Step 3: LAI validation module performs for each candidate:

    - Physical consistency check (does it conform to known physical laws?)

    - Constraint satisfaction check (does it satisfy manufacturability and other hard constraints?)

    - Mechanistic traceability (can a complete reasoning chain be generated?)

    ↓

Step 4: Validated candidates + reasoning chains output to user

    ↓
```

```
Step 5: Invalid candidates → analyze failure reasons → feedback to generation module

    ↓

Step 6: Generation module adjusts sampling distribution based on feedback → enters next iteration
```

The core innovation of this architecture is: the generation model handles "breadth," while LAI handles "depth"—the generation model rapidly explores the vast design space, while LAI provides deep mechanistic insight and trustworthy validation at critical nodes.

6. Case Demonstrations

6.1 Case 1: Inverse Design of Mechanical Metamaterials

Scenario: Designers require a mechanical metamaterial with both high strength and high energy absorption for aircraft crash energy-absorbing structures.

The Dilemma of Traditional Methods: There is a classic "trade-off relationship" between strength and energy absorption—increasing strength typically means reducing deformation capacity, thereby reducing energy absorption. A pure generative model might produce a "compromised" structure within the training data distribution, but cannot explain how this compromise was achieved or guarantee reliability under extreme conditions.

LAI Reasoning Process:

1. The system receives target set T = {high strength, high energy absorption}.
2. Activates High-Strength-Root and Energy-Absorption-Root.
3. The system identifies an inhibits relationship between the two Morpho-Roots—this is the strength-toughness trade-off explicitly represented at the Morpho-Root level.
4. The system searches for a third type of Morpho-Root that can mitigate this inhibitory relationship. Hierarchical-Structure-Root is identified as capable of partially decoupling this conflict by optimizing strength and toughness at different scales.
5. The system outputs the reasoning chain:

```
Target: High Strength + High Energy Absorption

    ↓ (conflict detected)

Strength-Root ⊥ Energy-Absorption-Root

    ↓ (resolution path found)

Hierarchical-Structure-Root

    ↓ (enables)

Nano-scale: Precipitation-Strength-Root
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Micro-scale: Cell-Buckling-Absorption-Root

    ↓ (validates)

Feasible Hierarchical Metamaterial Design
```

The system passes the reasoning chain to the generation module, which samples specific multi-level structural parameters under constraints.

Key Value: Designers receive not only a structure, but also the complete trade-off justification—why this structure can simultaneously achieve strength and toughness, and under what conditions this trade-off is valid.

6.2 Case 2: Inverse Design of Programmable Metamaterials

Scenario: Designers require a programmable metamaterial that responds to temperature stimulation for 4D printing self-deforming structures.

LAI Reasoning Process:

1. The system receives the target "temperature-responsive programmable deformation."
2. Activates Thermal-Response-Root.
3. Associates via couples_with to Shape-Memory-Root (shape memory effect is the classical mechanism for temperature-responsive deformation).
4. Further associates via requires to Multi-Material-Interface-Root (multi-material interfaces are the structural foundation driving the shape memory effect).
5. Checks via constrained_by to Manufacturability-Constraint-Root (manufacturability of multi-material interfaces).
6. Outputs the complete design blueprint: material combination scheme (two materials with large differences in thermal expansion coefficients) + interface geometry design + 4D printing process parameter recommendations.

Key Value: The complete reasoning chain from "temperature response" to "shape memory" to "multi-material interface" to "manufacturability validation" enables designers to understand the physical basis of every design choice, rather than blindly accepting the model's output.

7. Challenges and Prospects

7.1 Knowledge Engineering Bottleneck

Challenge: Building a complete "Metamaterial Morpho-Root" system requires systematically encoding decades of accumulated physical knowledge in the metamaterials field into computable form. This is a massive knowledge engineering undertaking.

Potential Paths:

- **Extraction from classical literature**: Extract mature physical models from classical textbooks, reviews, and milestone papers in the metamaterials field as "meta-Morpho-Root" seeds.
- **Community collaboration model**: Drawing on the Wikipedia model, establish an open Metamaterial Morpho-Root knowledge base, jointly maintained and expanded by domain experts.
- **Human-AI collaboration tools**: Utilize large language models to semi-automatically extract candidate Morpho-Roots and relations from the vast literature, with expert review and validation.

Liu further applies the LAI framework to trustworthy design of structural materials under extreme conditions, proposing a Morpho-Root-based graph reasoning framework and implementation strategy. This work provides methodological reference for the construction of the Metamaterial Morpho-Root knowledge base [3]. The "Metamaterial Morpho-Root" system proposed in this paper can be further extended and implemented on the basis of the OpenMorpho prototype framework [10].

7.2 Computational Complexity Challenge

Challenge: As the Morpho-Root network expands, graph traversal-based reasoning may face combinatorial explosion problems.

Scale Estimation: Preliminary estimates suggest that at moderate scales (~10^3 Morpho-Root types, ~10^4 relation edges), exact reasoning based on graph traversal is computationally feasible. When the network expands to 10^5–10^6 nodes, the following strategies need to be introduced:

- **Graph Neural Network (GNN) approximate reasoning**: Represent the symbolic Morpho-Root network as a graph structure, using GNN message passing mechanisms to rapidly evaluate the potential effects of different Morpho-Root combinations.
- **MSE-guided pruning**: Use MSE metrics to dynamically prune the search space, focusing on high-value regions.
- **Hierarchical reasoning**: Perform reasoning at different abstraction levels of the Morpho-Root network, avoiding premature combinatorial explosion at detailed levels.

7.3 Experimental Validation Loop

Challenge: Design solutions generated by LAI reasoning ultimately require experimental validation. How to establish a complete closed loop from "reasoning" to "experiment" to "knowledge update"?

Potential Paths:

- **Integration with self-driving laboratories**: Directly pass LAI reasoning results to automated experimental platforms, achieving a closed loop of "design–fabrication–testing–feedback."
- **Proactive uncertainty querying**: When MSE indicates knowledge gaps, the system proactively requests specific experiments to fill those gaps.
- **Incremental learning**: Experimental validation results are encoded as new Morpho-Roots or as corrections to existing Morpho-Roots, enabling continuous evolution of the knowledge base.

Liu, from a paradigm perspective, critiques the "rootless" predicament in current materials agent research, pointing out that the fundamental problem is that the Token-based AI paradigm cannot provide stable semantic foundations for materials agents [4]. The LAI framework, through its "rooted" cognitive architecture of Morpho-Roots, provides explainable decision-making foundations for self-driving laboratories and agentic AI.

8. Conclusion

This paper systematically maps the Logographic AI (LAI) theoretical framework to the field of inverse metamaterials design, proposing the "Metamaterial Morpho-Root" system and a Morpho-Root-based graph reasoning framework. The main contributions include:

First, identifying the fundamental bottlenecks of current deep generative model-driven inverse metamaterials design—inexplicability, unguaranteed constraints, and inefficient use of physical knowledge—and placing this problem within the macro perspective of "Technology Capture."

Second, proposing the formal definition of "Metamaterial Morpho-Root" and the core Morpho-Root system, encoding mesostructural features, physical response laws, and design constraints in the metamaterials domain as computable structured cognitive units $\tau = (S, A, R)$.

Third, designing an MSE-guided inverse reasoning engine that achieves fully traceable reasoning from target properties to feasible structures, with zero-violation assurance of hard constraints.

Fourth, proposing a hybrid architecture integrating LAI Morpho-Root networks with deep generative models, achieving the organic unity of "efficient sampling" and "trustworthy validation."

Fifth, demonstrating the specific working methods and unique value of the LAI framework in inverse metamaterials design through two case studies: mechanical metamaterials and programmable metamaterials.

The core thesis of this paper is: the future of inverse metamaterials design lies not in training larger generative models, but in reconstructing AI's cognitive architecture—from "statistical fitting" to "mechanistic reasoning." The Morpho-Root paradigm of Logographic AI provides a feasible philosophical foundation and implementation path for this purpose. When AI can not only "generate" metamaterial structures, but also "explain" why it generates them, "justify" why the design is reasonable, and "guarantee" that all engineering constraints are satisfied, metamaterials design can truly transform from "black-box art" to "trustworthy engineering."

Shen Liu proposes the vision of "Civilization-Native Intelligence" (CNI), advocating that every civilization can extract its own "cognitive roots" from the structural features of its language. This work can be seen as a concrete practice of this vision in the field of materials science—encoding the physical knowledge of the metamaterials field into "Metamaterial Morpho-Roots," building an AI cognitive architecture rooted in materials physics.

We call upon scholars from the metamaterials, AI, and knowledge engineering communities to jointly participate in the community construction of the "Metamaterial Morpho-Root" knowledge base, systematically encoding humanity's physical understanding of metamaterials into computable, shareable, and evolvable cognitive primitives. This is not only a paradigm upgrade for inverse metamaterials design, but also a critical step for the entire field of materials informatics to transition from "data-driven" to "mechanism-driven."

Conflict of Interest Statement

The author is the original proponent of the Logographic AI (LAI) theory cited in this paper (Refs. [1][2][3][4]), and is also one of the developers of the OpenMorpho prototype system (Ref. [10]). The exposition of Logographic AI theory and related technical frameworks in this paper is based on the aforementioned publicly published academic papers, monographs, and open-source code.

The author declares that, apart from the above academic contributions, there are no other conflicts of interest that may affect the objectivity and impartiality of this research.

Author Contributions

Shen Liu is the sole author of this paper and completed all work including conceptualization, theoretical framework design, methodology design, manuscript writing, literature analysis, and case design.

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Data and Code Availability Statement

This paper is a theoretical construction and conceptual demonstration and does not involve new experimental data. The source code of the engineering concept validation prototype OpenMorpho cited in this paper is open-sourced on the GitHub platform (Ref. [10]), and readers can access and run the relevant demonstrations through this link.

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