ACCSCIENCE PUBLISHING

International Journal of AI for Materials and Design

COMMENTARY

Artificial intelligence-enabled acceleration and enhancement of 4D device printing

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Abstract

Artificial intelligence (AI) and machine learning (ML) are rapidly emerging as necessary computational paradigms for 4D device printing—the additive manufacturing of structures programmed to dynamically transform their shape, properties, or functions over time in response to external stimuli. Unlike standard 3D printing, which targets static geometric fidelity and steady-state structural properties, 4D printing involves solving a highly non-linear, path-dependent inverse problem across coupled material-geometry-process-stimulus spaces. This commentary presents the central argument that data-driven and physics-informed AI methods are not merely optional optimizations, but mandatory tools required to navigate the temporal multi-physics design space and make 4D printing deterministic, reproducible, and commercially viable. We clearly delineate between methods already empirically demonstrated (*e.g.*, forward surrogate neural networks, convolutional inverse design of metamaterials, active learning for material discovery, and melt-pool defect detection) and methods currently proposed (*e.g.*, autonomous closed-loop digital twins, physics-informed neural ODEs for long-term degradation, and certified explainable AI pipelines for clinical implants). Furthermore, we distinguish the evidence base for static 3D printing (focusing on relative density, void formation, and static residual stresses) from dynamic 4D printing (focusing on spatiotemporal deformation, phase transformation kinetics in shape-memory alloys, rate-dependent hydrogel swelling, and hysteresis). We highlight the unique challenges of 4D printing—specifically, non-linear multi-physics coupling, extreme computational cost, sparse spatiotemporal experimental data, inverse design non-uniqueness, and actuation drift—and demonstrate qualitatively how physics-informed neural networks (PINNs), active learning, deep generative models, and computer-vision digital twins solve these bottlenecks. Finally, we re-emphasize in our conclusion the transformative role of spatiotemporal AI in bridging lab-scale smart materials and production-grade 4D functional systems.

Keywords: 4D printing; Artificial intelligence; Machine learning; Inverse design; Stimuli-responsive materials; Additive manufacturing; Digital twins

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Citation: Brabazon D. Artificial intelligence-enabled acceleration and enhancement of 4D device printing. *Int J AI Mater Design*. doi: 10.36922/IJAMD026360032

Received: September 2, 2026

Revised: November 6, 2026

Accepted: November 6, 2026

Published online: November 18, 2026

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1. Introduction

Additive manufacturing has evolved beyond the creation of static three-dimensional (3D) objects toward four-dimensional (4D) printing, where additively manufactured

structures are programmed to alter their shape, mechanical properties, or functionality over time (t) upon exposure to external environmental stimuli such as thermal variation, magnetic fields, moisture, light, or pH shifts.[1-5] Designing and manufacturing functional 4D devices requires navigating an extraordinarily high-dimensional parameter space that couples material synthesis (*e.g.*, polymer crosslinking density, alloy stoichiometry, filler loading), spatial micro-architecture (*e.g.*, spatial deposition toolpaths, voxel-level anisotropy, multi-material interfaces), manufacturing process parameters (*e.g.*, laser volumetric energy density, print speed, shear rate), and time-varying external stimulus actuation profiles.[1,6-8] A tenant of this commentary is that that artificial intelligence (AI) and machine learning (ML), specifically physics-informed neural networks, deep generative models, active learning, and closed-loop digital twins, are not merely optional workflow enhancements, but fundamental computational paradigms required to realize deterministic, reproducible, and scalable 4D device printing. Conventional forward modeling techniques, such as finite element analysis (FEA) or multi-physics partial differential equation (PDE) solvers, are computationally prohibitive when applied iteratively to non-linear transient shape transformations, often requiring hours or days per iteration.[1,7] The inverse problem determining the precise spatial material distribution, local orientation, and stimulus trajectory required to achieve a target continuous dynamic morphing profile is intrinsically non-unique, ill-posed, and non-linear.[1,9] Standard numerical optimization paradigms fail in this domain due to combinatorial explosion and local minima entrapment.[1,9] To establish a clear state-of-the-art framework, this work critically distinguishes between methods already empirically demonstrated in the literature and methods theoretical/proposed for future implementation. Moreover, an explicit distinction is drawn between evidence pertaining to static 3D printing (*e.g.*, part relative density, void formation, steady-state process optimization) and dynamic 4D printing (*e.g.*, time-dependent shape evolution, phase transformation kinetics, rate-dependent swelling, and actuation hysteresis). By systematically examining the unique multi-physics challenges of 4D printing and providing qualitative evidence of AI-driven solutions, this commentary maps out a rigorous pathway from lab-scale demonstrations to industrial and clinical deployment.

2. AI for material exploration and selection for 4D printing

Materials suitable for 4D printing including stimuli-responsive hydrogels, shape-memory alloys (SMAs, such as NiTi), magnetoactive elastomers, and liquid crystal elastomers (LCEs) exhibit highly complex, non-linear constitutive behaviors and narrow processing windows.[3,8,10,11] Synthesizing and selecting materials for 4D printing requires optimizing both manufacturability during printing (*e.g.*, printability, shear-thinning rheology, melt stability) and dynamic response post-printing (*e.g.*, rapid actuation rate, high recovery stress, minimal fatigue).[6,10]

2.1. Demonstrated methods

Machine learning surrogate models have been successfully applied to accelerate material property prediction, formulation screening and additive manufacturing process optimisation. In gel-based additive manufacturing, machine learning algorithms (*e.g.*, Gaussian Process Regression, Random Forests, XGBoost) have been demonstrated to map polymer formulation ratios, crosslinking density, and nozzle shear rates directly to yield stress, storage modulus (G'), and post-printing swelling ratios (Q), achieving high predictive accuracies.[6] Active learning (AL) and Bayesian optimization (BO) frameworks, employing surrogate models and uncertainty-based acquisition functions, have demonstrated the potential to substantially reduce the number of experimental evaluations required for materials discovery and manufacturing process optimization. Deneault *et al.*[12] demonstrated the application of Bayesian optimization to additive manufacturing process parameters, while Lookman *et al.*[13] highlighted the effectiveness of uncertainty-guided adaptive sampling for targeted materials design. However, the magnitude of experimental savings depends on the optimization problem, parameter space, acquisition strategy and baseline method used for comparison. For metallic smart materials, experimental studies of NiTi SMAs produced by powder bed fusion–laser beam (PBF-LB) have established relationships between processing parameters, microstructure, phase transformation behavior and residual stresses.[10,11] More recently, Chapman *et al.*[14] demonstrated that supervised machine learning models combining PBF-LB process parameters with *in situ* infrared thermal monitoring data could predict NiTi part relative density with an R^2 of 0.91, increasing to above 0.92 using thermal histories from four or more deposited layers, providing a foundation for future closed-loop process control.

2.2. Proposed methods

Conversely, several advanced material discovery paradigms remain proposed rather than fully validated. These include physics-informed neural differential equations (Neural ODEs) capable of predicting multi-cycle thermomechanical fatigue, degradation, and creep in stimuli-responsive polymers without requiring extensive empirical phenomenological fitting.[9] Additionally,

generative diffusion models and generative adversarial networks (GANs) are proposed for the zero-shot inverse synthesis of novel multi-stimuli responsive block-copolymer formulations and multi-component SMA compositions tailored for custom activation temperatures.[9]

3. AI for design exploration and inverse design 4D architectures

The spatial design of 4D-printed devices extends far beyond conventional 3D topology optimization. While 3D design optimizes static load-bearing capabilities or thermal dissipation, 4D inverse design must specify the continuous 3D spatial layout of materials, voxel-level fiber or grain orientations, toolpath vectors, and local swelling/straining capacities required to achieve a dynamic, time-dependent target shape transformation $U^{\star}(x, y, t, z)$.[1,7,9]

3.1. Demonstrated methods

Deep learning architectures have demonstrated considerable potential for addressing complex inverse design problems. Ma *et al.*[7] developed a deep residual neural network to accelerate the design of tunable magneto-mechanical metamaterials, establishing relationships between structural design parameters and their mechanical responses under applied magnetic fields. Their work demonstrates the potential of deep learning to accelerate the design and optimization of magnetically responsive architectures relevant to 4D printing. Sun *et al.*[1] demonstrated a machine-learning-enabled framework for forward shape prediction and inverse design of thermally and moisture-actuated 4D-printed composite plates. Their deep residual neural network provided accurate predictions of the resulting deformed shapes while substantially reducing the computational effort compared with conventional finite element simulations. Furthermore, data-driven approaches have been demonstrated to optimize spatial multi-material distributions in soft robotic actuators, mapping spatial stiffness gradients to target bending trajectories.[4]

3.2. Proposed methods

Proposed frameworks in 4D architecture design aim to address multi-stimuli, reconfigurable morphing. Generative continuous spatial material grading networks are proposed to co-optimize material deposition profiles and temporal stimulus activation sequences simultaneously.[3,9] Furthermore, physics-informed generative diffusion models are proposed to enforce global kinematic compatibility and prevent self-intersection during extreme large-deformation shape morphing pathways.[9]

4. Quality monitoring and closed-loop control: 3D vs 4D systems

A critical distinction must be drawn between quality monitoring in standard 3D printing and quality control in 4D device printing.

4.1. Evidence for 3D printing (static quality control)

In static 3D printing, quality monitoring focuses on steady-state process parameter optimization, *in situ* melt-pool geometry tracking, high-speed pyrometry, and optical/acoustic sensing to detect microscopic voids, surface roughness, and density degradation.[15-18] Machine learning approaches have been applied to melt-pool monitoring data for defect detection and part-density prediction in PBF-LB processes. Mahato *et al.*[17] investigated the prediction of layer porosity in PBF-LB using regression machine learning models and features extracted from *in situ* pyrometer time-series data, while Monu *et al.*[18] compared statistical, data-driven and physics-informed machine learning models for predicting the relative density of PBF-LB–produced stainless steel components.

4.2. Evidence for 4D printing (dynamic spatiotemporal control)

Experimental studies of PBF-LB-produced NiTi have demonstrated that processing conditions influence microstructure, phase transformation behavior and residual stresses.[10,11] These findings highlight the importance of developing *in situ* monitoring and predictive modelling approaches capable of linking manufacturing conditions to the subsequent functional performance of 4D-printed NiTi devices. For hydrogels, machine learning has been investigated for predicting material properties and optimising formulation and printing parameters,[6] while Bayesian optimization has demonstrated the potential for adaptive process parameter selection in additive manufacturing.[13] However, the integration of vision-based *in situ* monitoring with machine learning for real-time control of hydrogel shape transformation remains an area requiring further experimental validation.

4.3. Proposed methods for 4D control

Proposed advancements center on closed-loop, fully autonomous digital twins. These systems are proposed to integrate multi-camera computer vision (tracking real-time spatiotemporal shape recovery during stimulus exposure) with reinforcement learning (RL) controllers.[2,3,13] The RL agent is envisioned to dynamically recalibrate external stimulus delivery (*e.g.*, adjusting near-infrared laser intensity or modulating magnetic field gradients) in real time to compensate for manufacturing

imperfections, thermal dissipation, or environmental noise during actuation.[2,3] Explainable AI (XAI) can enhance the interpretation of image-based datasets acquired during 4D printing, including optical images, infrared thermal maps and microscopy data. Techniques such as SHapley Additive exPlanations (SHAP), Local Interpretable Model-agnostic Explanations (LIME) and Gradient-weighted Class Activation Mapping (Grad-CAM) can identify image regions or features that influence machine learning predictions, helping researchers relate observed structural changes and defects to predicted material or device performance. Such approaches can improve model transparency, support validation and guide the development of more reliable image-based quality monitoring systems.[19]

5. AI-enabled predictive modelling of printed 4D device actuation

Predicting 4D actuation requires modeling transient, multi-physics dynamic responses, including shape recovery kinetics, generated actuation forces, response time, multi-stability, and cyclical actuation fatigue.[1,6,7]

5.1. Demonstrated methods

Data-driven surrogate models, particularly deep neural networks, have demonstrated considerable potential for predicting deformation and shape-changing behavior in 4D-printed active materials. Sun *et al.*[1] employed a deep residual neural network to predict the actuated shapes of 4D-printed composite plates, achieving high predictive accuracy ($R^2 = 0.995–0.999$), while Ma *et al.*[7] demonstrated deep-learning-based prediction of the global strain response of magneto-mechanical metamaterials under magnetic actuation. Machine learning has also been investigated for material formulation and process optimization in gel-based additive manufacturing,[6] although its application to predicting time-dependent actuation behaviour requires further validation. Physics-guided machine learning offers opportunities to incorporate governing physical relationships and constraints into predictive models, potentially improving their physical consistency and generalisation beyond the training data.[9]

5.2. Proposed methods

Proposed predictive paradigms include spatiotemporal physics-informed neural networks (PINNs) capable of solving high-dimensional non-linear thermo-viscoelastic and phase-field partial differential equations in real time.[9] These proposed operators aim to enable instant forward actuation prediction under arbitrary, continuous, unlearned stimulus schedules. Furthermore, explainable AI (XAI) frameworks, including SHAP, LIME and counterfactual explanations, could improve the interpretability of predictive models by identifying the contributions of material, processing and design parameters to predicted device performance. Such approaches may support model transparency, validation and regulatory assessment of patient-specific 4D-printed biomedical devices, including self-expanding vascular stents and dynamic tissue scaffolds, although their effectiveness and regulatory acceptance in these applications remain to be demonstrated.[3,20]

6. Conclusions

This commentary has critically established the fundamental premise that AI is an indispensable computational paradigm for 4D device printing. Unlike 3D printing which targets static structural integrity and defect-free geometry, 4D printing operates in a continuous spatio-temporal domain governed by non-linear multi-physics, path-dependent hysteresis, rate-dependent kinetics, and highly non-unique inverse mappings.

While empirical work has demonstrated forward surrogates, metamaterial inverse design, active material screening, and static 3D defect detection the transition to production-grade 4D manufacturing requires advancing proposed frameworks: closed-loop spatiotemporal digital twins, neural ODEs for long-term fatigue prediction, and certified explainable AI (XAI) pipelines. By integrating physics-informed learning, robust data stewardship, and real-time hardware-software control loops, AI will transform 4D device printing from empirical laboratory demonstrations into a deterministic, scalable technology for advanced biomedical implants, dynamic soft robotics, and adaptive industrial structures.

Acknowledgments

None.

Funding

This publication has emanated from research supported by Research Ireland under Grant Number 21/RC/10295_P2 and is co-funded under the European Regional Development Fund.

Conflict of interest

The author declares no competing interests.

Author contributions

This is a single-authored article.

Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Availability of data

Not applicable.

AI tools statement

The author acknowledge the use of Google Gemini 4 (Google LLC, USA) for language and grammatical refinement. All text was manually reviewed and verified by the author to ensure technical precision and clarity.

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