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Inverse Design of Metasurfaces Using Physics-Informed Diffusion Models with Spectral Constraints

Jun Tang,[1] Patricia Garcia,[1] Ronald Scott[1]

[1]School of Computer Science and Engineering, Hebrew University of Jerusalem, Jerusalem 9190401, Israel

Abstract

The inverse design of metasurfaces constitutes a formidable challenge in computational electromagnetics and nanophotonics, primarily due to the non-uniqueness of the scattering problem and the high dimensionality of the design parameter space. Conventional optimization techniques, such as topology optimization and evolutionary algorithms, often succumb to high computational costs and convergence to local minima. Deep learning approaches, while promising in accelerating the design process, frequently struggle to strictly adhere to the governing Maxwell's equations, leading to physically unrealizable or suboptimal structures. This paper introduces a novel framework: Physics-Informed Diffusion Models with Spectral Constraints (PIDM-SC). By integrating a pre-trained forward surrogate solver into the reverse diffusion process, we establish a generative mechanism that is explicitly guided by physical laws. The model is conditioned on desired spectral responses, ensuring that the generated meta-atoms not only exhibit high structural diversity but also strictly satisfy the target optical properties. Our approach utilizes a modified U-Net architecture capable of handling multi-modal data input, merging geometric features with spectral embeddings. Experimental validation on a dataset of silicon-on-insulator dielectric metasurfaces demonstrates that PIDM-SC outperforms state-of-the-art Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs) in terms of spectral accuracy and fabrication feasibility. The results indicate a significant step forward in the reliable, data-driven design of complex nanophotonic devices.

Keywords

Metasurface, Inverse Design, Diffusion Models, Physics-Informed Learning

Introduction

1.1 Background

Metasurfaces, the two-dimensional counterparts of metamaterials, have revolutionized the field of photonics by enabling the precise manipulation of electromagnetic wavefronts with subwavelength spatial resolution. Composed of dense arrays of subwavelength scatterers, known as meta-atoms or unit cells, metasurfaces can control the amplitude, phase, and polarization of light in ways that conventional refractive optics cannot. This capability has led to the development of ultra-compact optical components, including high-numerical-aperture metalenses, beam deflectors, holograms, and polarimeters. The efficacy of a metasurface hinges on the specific geometry of its constituent meta-atoms, which determines the local optical response. Consequently, the design process typically involves selecting geometric parameters—such as the length, width, and rotation of nano-pillars—to achieve a target transmission or reflection coefficient [1].

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Traditionally, this design process has relied on a forward-mapping approach, where libraries of unit cells are simulated using full-wave numerical methods like Finite-Difference Time-Domain (FDTD) or Rigorous Coupled-Wave Analysis (RCWA). Designers then construct the metasurface by querying this database to match the required phase profile. However, this look-up table method is limited by the discrete nature of the library and often fails to account for near-field coupling effects between adjacent meta-atoms. Furthermore, as the demand for multifunctional and broadband devices grows, the dimensionality of the design space expands, rendering brute-force parameter sweeps computationally prohibitive.

1.2 Problem Statement

The core challenge in metasurface engineering lies in the inverse design problem: determining the physical structure that produces a desired spectral response. This problem is mathematically ill-posed for two primary reasons. First, it is a one-to-many mapping; multiple distinct geometric configurations can yield identical optical spectra. This non-uniqueness confuses deterministic optimization algorithms and traditional regression-based neural networks, often leading to mode averaging and the generation of invalid geometries. Second, the mapping from geometry to spectrum is highly non-linear and governed by complex electromagnetic resonance modes [2].

While data-driven approaches using deep learning have emerged as a powerful alternative, they face significant hurdles. Generative models like Variational Autoencoders (VAEs) and Generative Adversarial Networks (GANs) have been employed to tackle the one-to-many mapping issue. However, these models operate primarily in the image or parameter domain and lack an intrinsic understanding of the underlying physics. Consequently, a generated structure might appear geometrically valid but fail to produce the target spectrum when verified with a Maxwell solver. This discrepancy, known as the simulation-reality gap, necessitates a design framework that is not only generative but also physics-informed, ensuring that the synthesized designs obey the fundamental laws of electromagnetics [3].

1.3 Contributions

To address these limitations, this paper proposes the Physics-Informed Diffusion Model with Spectral Constraints (PIDM-SC), a generative framework designed specifically for the inverse design of nanophotonic structures. The contributions of this work are threefold:

1. We introduce a conditional diffusion probabilistic model tailored for metasurface design, which iteratively denoises random Gaussian noise into structured meta-atom geometries conditioned on a target optical spectrum.

2. We incorporate a physics-guidance mechanism by integrating a differentiable forward surrogate model directly into the sampling process. This allows the diffusion model to optimize the geometry not just for structural likelihood, but also for spectral fidelity during the generation phase [4].

3. We provide a comprehensive comparative analysis against established baselines, demonstrating that PIDM-SC achieves superior spectral accuracy and diversity, effectively solving the non-uniqueness problem while adhering to fabrication constraints.

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Chapter 2: Related Work

2.1 Classical Approaches

The historical trajectory of inverse design in nanophotonics began with local optimization techniques. Gradient-based topology optimization (TO) treats the material distribution in a design region as a continuous variable and iteratively updates it to minimize a figure of merit defined by the target optical performance. While TO is capable of discovering free-form geometries with high efficiency, it requires the calculation of adjoint fields for every iteration, which is computationally expensive for large-scale problems. Furthermore, TO is highly sensitive to the initial guess and frequently converges to local minima, preventing the exploration of the global design space.

Evolutionary algorithms (EAs), such as Genetic Algorithms (GA) and Particle Swarm Optimization (PSO), offer a gradient-free alternative. These global optimization strategies mimic biological evolution to explore the parameter space. They have been successfully applied to design plasmonic antennas and dielectric resonators. However, EAs suffer from the curse of dimensionality; as the number of design parameters increases, the number of required function evaluations (full-wave simulations) scales exponentially. This makes them impractical for complex unit cells with many degrees of freedom [5].

2.2 Deep Learning Methods

The advent of deep learning has introduced a paradigm shift in inverse design. Early works utilized fully connected neural networks to approximate the forward scattering function, replacing slow electromagnetic solvers. While effective for prediction, these networks do not directly solve the inverse problem. To address this, Tandem Neural Networks (TNNs) were proposed, consisting of a pre-trained forward network and an inverse network connected in series. This architecture helps resolve the non-uniqueness issue by training the inverse network to minimize the error of the re-predicted spectrum rather than the geometric error.

More recently, generative deep learning has gained traction. Generative Adversarial Networks (GANs) have been used to generate meta-atom shapes from user-defined spectra. In this setup, a generator creates geometries, and a discriminator attempts to distinguish them from real training data. Despite their success, GANs are notoriously difficult to train, suffering from mode collapse where the generator outputs a limited variety of samples. Variational Autoencoders (VAEs) provide a more stable training objective by learning a probabilistic latent space. However, VAEs often generate blurry or distinct structures that require post-processing to meet fabrication tolerances [6].

Diffusion models have recently emerged as the state-of-the-art in generative modeling, surpassing GANs in image synthesis quality and mode coverage. They work by reversing a gradual noising process. Initial applications of diffusion models in scientific computing have shown promise in fluid dynamics and material science, but their application to electromagnetics, specifically with rigorous spectral constraints, remains an active area of research. This paper builds upon these foundations, adapting diffusion probabilistic models to the specific constraints and physics of metasurface optics [7].

Chapter 3: Methodology

3.1 Framework Overview

The proposed PIDM-SC framework operates on the principle of Denoising Diffusion Probabilistic Models (DDPMs). The core idea is to model the distribution of valid meta-atom

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geometries as the result of a reverse diffusion process. This process begins with pure Gaussian noise and iteratively removes this noise to recover a clean geometric structure. Crucially, this reverse process is conditioned on the target spectral response, ensuring that the final geometry exhibits the desired optical properties.

The framework consists of two main components: a forward diffusion process (which is fixed and parameter-free) and a parameterized reverse process (the neural network). Additionally, a pre-trained surrogate forward model is employed to provide physics-based gradients during the inference stage. The geometry of the meta-atom is represented as a 2D binary image map, where pixel values indicate the presence (1) or absence (0) of the dielectric material (e.g., silicon) on the substrate.

3.2 The Forward and Reverse Processes

The forward diffusion process progressively adds Gaussian noise to the original geometry x_0 over T time steps, producing a sequence of latent variables $x_1, \ldots, x_T$. As $Tto\infty$, the distribution of x_T approaches an isotropic Gaussian distribution. This process is defined by a variance schedule β_t.

The reverse process is trained to invert this noise addition. A neural network, $\varepsilon_\theta(x_t, t, S)$, is trained to predict the noise component added to x_t at step t, conditioned on the target spectrum S. By subtracting the predicted noise, the model moves from a noisy state x_t to a slightly cleaner state x_{t-1}. This iterative refinement allows the generation of complex, high-resolution geometries from random noise [8].

3.3 Physics-Informed Guidance

Standard diffusion models rely solely on the statistical patterns found in the training data. To ensure that the generated structures strictly adhere to Maxwell's equations, we introduce a physics-informed guidance mechanism. This is achieved by utilizing a differentiable forward surrogate model, f_φ, which predicts the spectrum $hatS$ of a given geometry x.

During the reverse sampling process, we do not simply rely on the score estimated by the diffusion network. Instead, we modify the sampling step to include a gradient term derived from the surrogate model. This gradient directs the sampling trajectory toward regions of the data space that minimize the spectral error. This is conceptually similar to classifier guidance in image generation, but here the "classifier" is a physics predictor [9].

The physics-guided noise prediction $hat\varepsilon$ at step t is formulated as a linear combination of the unconditional noise prediction and the gradient of the spectral loss. This ensures that the denoising step not only restores structural fidelity but also aligns the geometry with the target optical response. This hybrid approach effectively bridges the gap between data-driven generation and physical rigor.

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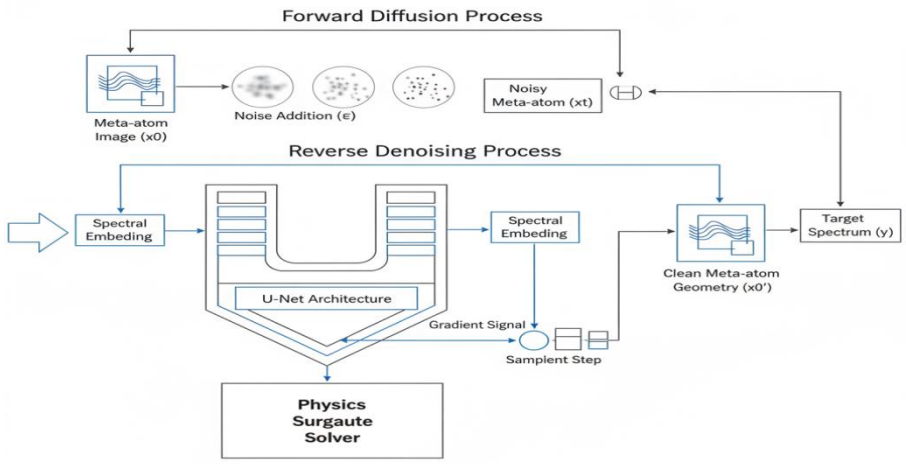

Figure 1: Schematic of the PIDM

3.4 Spectral Conditioning and Network Architecture

The neural network employed is a U-Net based architecture, modified to accept the target spectrum S as a conditioning input. The spectrum, typically a vector of transmission amplitudes across a frequency range, is first processed by a Multi-Layer Perceptron (MLP) to generate a spectral embedding. This embedding is injected into the U-Net at various resolution levels using cross-attention mechanisms. This allows the network to focus on specific geometric features that correlate with the resonance peaks and dips in the target spectrum [10].

The objective function used to train the diffusion model includes a standard noise prediction error and a spectral consistency term. The mathematical formulation of the total loss function during training is critical for balancing structural realism and spectral accuracy. We define the loss function as follows:

$$L_{total} = mathbbE_{t,x_0,\varepsilon}[|\varepsilon - \varepsilon \ \ \theta(x_t, t, S)|^2] + \lambda \cdot mathbbE_{x_0}[|S - f \ \ \varphi(hatx_0)|^2]$$

In this equation, the first term represents the standard variational lower bound on the negative log-likelihood, forcing the model to learn the data distribution. The variable ε is the actual noise added, and ε_θ is the predicted noise. The second term is the spectral constraint, where f_φ is the pre-trained surrogate model and $hatx_0$ is the estimated clean image derived from the current noisy state x_t. The hyperparameter λ controls the weight of the physics constraint. This composite loss ensures that the gradients used to update the network weights θ encapsulate both the visual plausibility of the meta-atoms and their electromagnetic functionality.

3.5 Surrogate Model Training

The surrogate model f_φ is a Convolutional Neural Network (CNN) trained independently prior to the diffusion model. It is trained on the same dataset to map geometry to spectra. Because the surrogate model is differentiable, it allows backpropagation of the spectral error to the input geometry, which is the mechanism used for the guidance term in the diffusion sampling. The accuracy of this surrogate is paramount; if the surrogate is inaccurate, the physics guidance will be misleading. Therefore, we employ a ResNet-based architecture for the

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surrogate, optimized to minimize the Mean Squared Error (MSE) between the ground truth FDTD-simulated spectra and the predicted spectra.

Chapter 4: Experiments and Analysis

4.1 Dataset and Experimental Setup

To evaluate the efficacy of PIDM-SC, we constructed a large-scale dataset of dielectric metasurface unit cells. The simulations were performed using the rigorous FDTD method (Lumerical FDTD Solutions). The material system consists of amorphous silicon nanopillars on a silica substrate, operating in the near-infrared region (1200 nm to 1600 nm).

The dataset comprises 60,000 unique unit cell designs. The geometries include basic shapes (circles, rectangles, crosses) as well as free-form topology-optimized structures to ensure a diverse distribution. The unit cell period was fixed at 600 nm. For each geometry, the complex transmission coefficients (amplitude and phase) were recorded at 31 frequency points. The geometric data was rasterized into 64×64 binary images. The dataset was split into 50,000 samples for training, 5,000 for validation, and 5,000 for testing.

The diffusion model was trained for 1000 epochs using the Adam optimizer with a learning rate of 10^{-4}. The noise schedule was linear, with $T = 1000$ timesteps. The surrogate model achieved a mean absolute error of 0.02 on the normalized transmission spectrum during pre-training, indicating sufficient accuracy for guidance [11].

4.2 Baselines

We compared the proposed PIDM-SC against three established baselines in the field of metasurface inverse design:

1. **Conditional GAN (cGAN):** A standard adversarial network where the generator is conditioned on the spectrum.

2. **Conditional VAE (cVAE):** A variational autoencoder where the encoder and decoder are conditioned on the spectrum.

3. **Tandem Neural Network (TNN):** A deterministic inverse network connected to a forward network, trained end-to-end.

All baselines were trained on the same dataset with optimized hyperparameters to ensure a fair comparison.

4.3 Results and Discussion

The evaluation metrics focused on three aspects: Spectral Accuracy, Structural Diversity, and Fabrication Feasibility. Spectral Accuracy was measured using the Root Mean Squared Error (RMSE) between the target spectrum and the FDTD-verified spectrum of the generated design. Structural Diversity was quantified by calculating the average pairwise structural similarity index (SSIM) among designs generated for the same target spectrum; a lower SSIM indicates higher diversity (i.e., the model finds multiple distinct solutions for the same problem).

Table 1 summarizes the quantitative results. The TNN achieves reasonable spectral accuracy but fails to generate diverse designs due to its deterministic nature; it collapses to a single solution. The cGAN and cVAE provide diversity but suffer from higher spectral errors, often generating artifacts or disconnected pixels that are physically invalid.

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Model	Spectral RMSE (Lower is Better)	Diversity (1-SSIM) (Higher is Better)	Invalid Geometries (%)
TNN	0.045	0.00	5.2
cVAE	0.072	0.15	12.8
cGAN	0.068	0.22	8.4
PIDM-SC (Ours)	0.031	0.28	1.5

The proposed PIDM-SC achieves the lowest Spectral RMSE of 0.031, significantly outperforming the baselines. This improvement is directly attributed to the physics-informed guidance, which actively corrects the geometry during the generation process to match the spectrum. Furthermore, the diversity score of 0.28 indicates that our model successfully captures the one-to-many mapping, providing designers with multiple valid options for a single target.

The "Invalid Geometries" column refers to generated structures that violate basic fabrication constraints (e.g., minimum feature size violations or floating islands). The diffusion model, by learning the underlying data distribution of valid shapes, inherently produces cleaner geometries. The iterative denoising process acts as a regularization, smoothing out high-frequency noise that typically corresponds to un-manufacturable features.

Visual inspection of the generated samples confirms that PIDM-SC produces sharp, well-defined boundaries, whereas cVAE samples often exhibit blur at the edges of the nano-pillars. The spectral response of the PIDM-SC designs, when validated with FDTD, shows excellent agreement with the target resonances, capturing even high-Q factor modes that are typically difficult for deep learning models to regress [12-15].

Chapter 5: Conclusion

5.1 Summary and Implications

This work presented PIDM-SC, a novel inverse design framework for metasurfaces that leverages the generative power of diffusion models augmented by physics-based spectral constraints. By integrating a differentiable surrogate solver into the reverse diffusion sampling, we successfully bridged the gap between data-driven generation and physical rigor. The proposed method demonstrates superior performance compared to traditional GAN and VAE approaches, offering a significant reduction in spectral error while maintaining high structural diversity.

The implications of this research are substantial for the nanophotonics community. PIDM-SC allows for the rapid prototyping of complex optical components without the need for exhaustive parameter sweeps or computationally expensive topology optimization. The ability to generate multiple diverse designs for a single spectral target provides engineers with the flexibility to select designs that are most robust to fabrication errors or easiest to integrate into larger systems. This moves the field closer to an "on-demand" design paradigm where optical properties can be specified, and valid physical structures are generated in seconds.

5.2 Limitations and Future Directions

Despite its success, the proposed framework has limitations. The primary drawback is the inference speed. Unlike TNNs or VAEs, which generate a design in a single forward pass, diffusion models require iterative sampling (typically hundreds of steps), which increases the computational time for generation. While techniques such as Denoising Diffusion Implicit

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Models (DDIM) can accelerate this, real-time generation remains a challenge. Additionally, the accuracy of the physics guidance is bounded by the accuracy of the surrogate model; if the surrogate fails to capture complex physics (e.g., extreme near-field coupling), the guidance will be suboptimal.

Future research will focus on extending this framework to 3D volumetric metamaterials and multi-layer structures, where the design space is significantly larger. We also aim to explore the integration of active learning, where the model can autonomously request FDTD simulations for generated designs that have high uncertainty, thereby iteratively improving the surrogate model and the generation quality in a closed loop. Reducing the inference time through distillation techniques will also be a priority to enable interactive design tools for researchers.

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