Artificial Intelligence to Accelerate the Design and Discovery of Intelligent Metamaterials: The Way Forward

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Abstract

Metamaterials are artificially structured electromagnetic composites that have applications across a wide spectrum of verticals due to its unique ability to control electromagnetic waves at will. The emergence of a new class of intelligent, reconfigurable metamaterials is expected to play crucial roles in devices for next generation communication systems and transformational optics. Their design process relies heavily on time-consuming, computationally intensive, iterative numerical full wave simulations that require significant domain expertise. The recent proliferation of deep learning (DL) frameworks for accelerating the design and discovery of metamaterials have been shown to drastically reduce design times as well as computational expense with considerably reduced reliance on domain knowledge. However, robust inverse design models for active, reconfigurable metamaterials are still an open problem which is expected to generate exciting research problems and ultimately accelerate the adoption of these versatile electromagnetic composites into real-world scenarios. In this position paper, we briefly review some popular DL frameworks for solving the inverse problem in electromagnetic composites in general and provide recommendations for extending the same for active metamaterials.

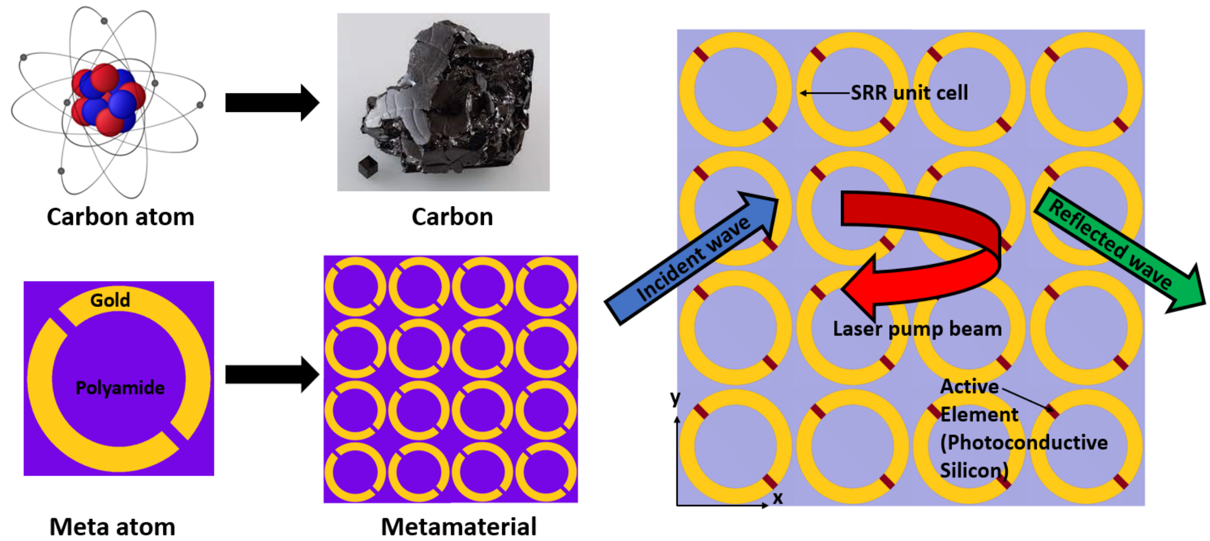
Introduction

Metamaterials and metasurfaces (planar, ultra-thin metamaterials) are artificially engineered composites that can manipulate electromagnetic (EM) waves in unconventional ways, thereby achieving extraordinary phenomena such as negative refraction, cloaking etc. (Pendry 2000; Cai 2007), which are not supported by naturally occurring materials. Metasurfaces in particular, consist of 2-dimensional arrays of fundamental building blocks called "meta-atoms" (Fig. 1(a)), having physical dimensions smaller than the operating wavelength. Electromagnetic responses and wave-matter interactions are dictated by the size, shape and geometry of these meta-atoms rather than properties of their constituent materials. The ability to control EM waves in unconventional ways along with their reduced physical size and lesser environmental footprints, have made metamaterials an attractive choice for replacing conventional electro-optic components in a wide variety of systems. Examples include transformational 'meta' lenses that are essentially planar films that can replace conventional bulky, expensive lens assemblies in cameras and smartphones and metamaterial-based antennas in place of conventional phased arrays in ultra-massive MIMO systems.

There are two major drawbacks that limit the penetration of metamaterials into real-world scenarios today; the first has to do with the fact that once a conventional (or passive) metamaterial is fabricated, its functionalities cannot be altered and therefore, its EM response cannot be tuned. This becomes a bottleneck for applications which require transient responses to accommodate state changes. This limitation is addressed by integrating an active element into the composite that responds to external stimuli (typically in the form of voltage/current, optical or thermal signals) thereby changing the state of the meta atoms post- fabrication. This new class of metamaterials (Nemati 2018) is termed as 'intelligent' or 'active' or 'programmable' or 'reconfigurable' metamaterials (these terms can be used interchangeably)(Fig. 1(b)). In the context of wireless communication systems, the term 'Reconfigurable Intelligent Surfaces (RIS)' is most widely used. The second major drawback is the lack of versatile, data-driven rapid prototyping tools for metamaterials which is a major impediment to the mass production of EM composites. Both issues can significantly benefit from robust inverse models.

Once metamaterial structures are designed, their responses are typically calculated by iterative, numerical full wave simulations such as finite difference time-domain (FDTD) and finite element method (FEM). However, this method requires significant experience and expertise of the designer and is an inefficient and time-consuming approach, especially for more complex structures. Recently, DL based frameworks have gained considerable research interest in the structural design (inverse design) and response prediction (forward design) of passive metamaterials:

- **Forward design:** In forward design models, a neural network is employed to predict the spectral response (amplitude, phase), scattered electric field distribution, focal length (for metalens) etc. for a given set of geometrical and/or material parameters as input.
- **Inverse design:** In inverse design, a neural network is employed to predict the geometrical and/or material parameters of the metamaterial from the response, given as



(a) (b)

Figure 1: (a) Illustration of a meta-atom and metamaterial with respect to conventional materials and their atoms (b) Reconfigurable metamaterial (Brown region is the active element - photoconductive silicon; external laser beams control the frequency at which maximum reflection occurs)

input to the network.

Inverse design is practically more useful and has gained more popularity as it can enable the user to obtain the most optimized structure that will generate the given response in very less time and without the requirement of domain expertise. Open problems in this field lies in - 1. Developing DL frameworks that can inversely design the structure of active metamaterials, particularly generating the most optimal design while taking the external control signal into account and 2. Employing DL to enable mass manufacturing of metamaterials.

The paper is organized as follows - Section II briefly describes the current metamaterial market and the technologies where they will become a key part in coming years. Section III reviews different DL frameworks being used to solve inverse problem in the metamaterial domain. Section IV provides some possible recommendations to tackle the two most challenging problems in this field - How DL can accelerate the inverse design of reconfigurable metamaterials and aid to enable mass manufacturing of metamaterials.

Metamaterial Industry and Technologies of the Future

In 2021 the metamaterial market was valued at USD 305 million, which is expected to reach USD 1457 by 2026, growing at 36% CAGR. This growth is attributed to the rapid adoption of metamaterials across various industries - Telecommunication, aerospace, defense, automotive, security, consumer electronics, energy and healthcare (Fig. 2), spanning over wide range of applications including antennas, flat lenses, sensors, solar absorbers, radars, etc. At present, the key market players are - Kymeta Corporation, Metamaterial Technologies Inc., Echodyne Inc., Plasmonics Inc., Lumotive LLC etc. In coming years, metamaterial based antennas and engineered flat-lenses are expected to fuel the growth in this field, owing to their tremendous applications in next generation wireless communication systems - Terahertz communication - 6G and beyond (Samsung 2020) and imaging technologies (Chen 2018) - sub-diffraction imaging, AR/VR respectively.

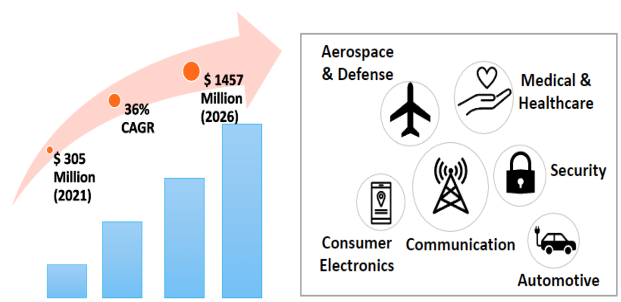


Figure 2: Metamaterial market size and key verticals

However, to implement efficient metamaterial based components at large scale in the above mentioned domains, it is crucial to migrate from passive metamaterial based devices to active or programmable metamaterials.

Passive Metamaterial Inverse Design Using DL

Prior to deep learning (DL) based techniques, evolutionary optimization algorithms like Particle swarm optimization (PSO), Genetic algorithm (GA) and Ant colony optimization (ACO) were widely used for inverse design of meta-

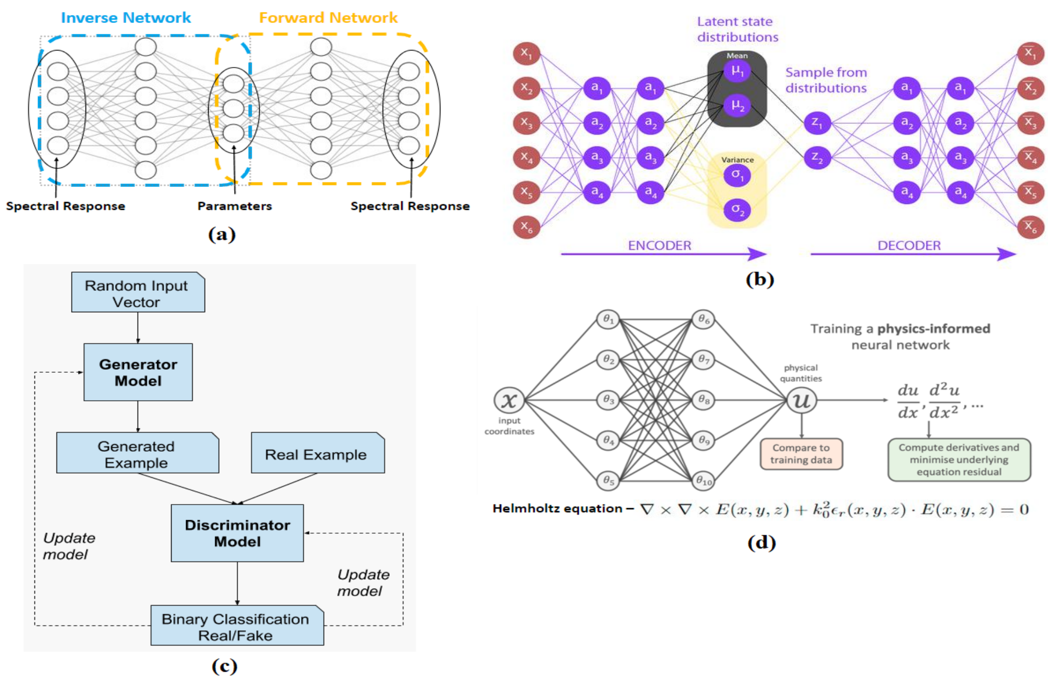


Figure 3: (a) Tandem network (b) Variational Autoencoder *(Source - www.geeksforgeeks.org/variational-autoencoders/)* (c) Generative Adversial Network *(Source - machinelearningmastery.com/what-are-generative-adversarial-networks-gans/)* (d) Physics Informed Neural Network *(Source - benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/)*

surfaces (Campbell 2019). However, as the parameter space of materials, geometries and the complexity of meta-atom structures increased, the computational time and power of these algorithms grew exponentially. To tackle this ever increasing design complexities of metasurfaces in reasonable time and computation power, DL based methodologies for inverse design have been employed.

Over the past few years, ANNs and DNNs have made remarkable progress in accelerating the design of metamaterials and nanophotonic structures in terms of computational time (Ma 2018; An 2019; Jiang 2021). In this domain, a trained neural network approximately predicts the solution of Maxwell's equations, which otherwise requires solving them iteratively through numerical methods like FDTD or FEM. During a forward prediction, the network maps the structural and material parameters to its response. During an inverse prediction, it maps the response to the geometry and material properties of the metasurface. However, there are significant challenges which limit the application of simple ANN-based models in inverse prediction of metasurfaces:

- **One-to-many mapping problem -** A desired EM response can be achieved by more than one set of structural and material parameters. Hence, the parameters inversely predicted by the network may not correspond to the optimal design.
- They perform usually very well within the range of their training data, but often generalize rather poorly to cases outside the parameter range.
- Limits the inverse design to one solution per design target, rendering inaccessible possible multiple solutions to a given problem.
- Require large number of datasets to train, yet acts as a universal function approximator - unable to develop a deeper "understanding" of the underlying physics.

The above challenges can be addressed by employing more sophisticated neural network architectures as discussed below (Raissi 2019; Wiccha 2021; Ma 2022).

Tandem Networks

Tandem networks (Fig. 3(a)) are a combination of Forward Neural Network (FNN) and Inverse Neural Network (INN). Once the network is trained, the FNN can predict the spectral responses accurately for a given set of geometrical and material parameters. The INN takes in the target spectral responses and gives the prediction of the possible structural and material parameters. The idea behind tandem networks is to train the FNN first, and then connect the output of INN to this pre-trained FNN and use the forward prediction loss to supervise the learning of INN. Using this two-step training, tandem networks circumvent the one-to-many mapping issue by enforcing the INN to converge to only one possible solution suggested by FNN.

Variational Autoencoders (VAEs)

VAEs (Fig. 3(b)) are generative models that can stochastically output multiple different predictions given the same input. It consists of three networks, namely - recognition network, generation network and conditional prior network.

During the training process, the recognition network learns to encode the structures and its corresponding response together into latent variables, whereas the generation network learns to decode the structures from the latent variables based on the conditional responses. The latent variables follow a normal distribution and they enable VAEs to generate multiple predictions when decoding from different latent variables. The conditional prior network provides the reconstruction of structures that are useful during inverse prediction.

Generative Adversarial Networks (GANs)

Like VAEs, GANs (Fig. 3(c)) are also a type of generative model, consisting of two networks - the generator network that generate structures based on the random variables and the spectral response; and the critic network that attempt to distinguish if a structure is from the dataset or from the generator network. The idea of GANs is based on the game theory, where the generator network always learns to generate structures that are distributed as close as possible to the test dataset, in order to fool the critic network; while the critic network always learns to distinguish the generated structures from real structures. Both VAEs and GANs overcome the limitation of inverse design giving one solution per design target.

Physics Informed Neural Network (PINN)

Raissi etal. in 2019 presented a new DL framework to solve forward and inverse problem for physics based applications involving partial differential equations (PDE) (Fig. 3(d)). The loss function of a PINN is defined by the PDE that governs the physics of the phenomenon we are modelling. For example, in nanophotonics and metamaterials, the loss function is the Helmholtz equation, which is derived from Maxwell's equations that govern the wave-matter interaction. PINNs not only learn the underlying physics of the problem, these networks can also be trained by using a single dataset. As a result, they have gained significant research interest in recent times.

Open Challenges and Future Scope

Unlike passive metamaterials, inverse design of reconfigurable metamaterials posses an additional challenge of predicting the value of external control signal (bias) along with the geometrical and material parameters - such that the combination has the most optimal design and generates the exact desired response. The problem becomes even more complex when there is both spatial and temporal variation of the states of each meta-atoms in the structure. For example, in a metalens, a particular spatial distribution of the phase profile focuses the light at focal length f_1. To inversely design it, the model has to predict the structural properties as well as the spatially varying state of the meta-atoms (due to the bias) that will give rise to that phase profile. When the focal length shifts to f_2, the phase profile and hence the spatial variation of each meta-atoms' state will now change in temporal domain, which also needs to be addressed by the DL model. As the availability of large number of datasets is a major problem in this domain, one solution to inversely design active metamaterials is by using physics based models. To tackle more complicated problems involving sequential data in time or space (spectral response or electric field distribution), implementing more complex DL architectures like LSTMs along with a physics-based loss functions involving equations that govern the underlying physics is recommended. Optimization algorithms have recently been used for designs for fabrication for semiconductor foundries to produce designs that can be reliably fabricated at large scales (Piggott 2020). As metamaterial components can also be fabricated by the techniques used for silicon photonics - Deep reactive ion etching, Lithography, Laser micromachining etc. (Tao 2008; Ako 2020), it is promising to explore DL frameworks over traditional optimization algorithms that can generate realistic, 'achievable' metamaterial structures which also account for variabilities in fabrication tolerances, for scaling up manufacturing .

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