Synergy of Machine Learning and Mie-tronics: Tailoring Resonant Response of Meta-atom on Demand

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Abstract

Optical metasurfaces are engineered 2D electromagnetic structures enabling flat optical elements with properties not readily found in nature. Their unit cells, meta-atoms, usually are represented by a set of electric and magnetic multipoles. All-dielectric-based metasurfaces have recently attracted significant attention owing to their virtually lossless transmission properties at optical frequencies. A majority of reported dielectric metamaterials are composed of relatively simple meta-atoms such as spheres, cubes, and cylinders, whose electromagnetic response is dominated by the electric dipole. However, magnetic dipoles and higher-order multipoles may enable new optical properties and functionalities, including directional scattering, beam steering, and new frequency generation. Despite impressive progress in the field of optical metamaterials and nano-fabrication technologies, engineering meta-atoms that support such higher-order resonances is still challenging. Here, we demonstrate that designed titanium dioxide meta-atoms can enable dominant magnetic dipole response. We apply a machine-learning model to predict a meta-atom shape with a strong magnetic dipole resonant mode at the operating wavelength of 750 nm. Using finite-element-based numerical simulations implemented in COMSOL Multiphysics, we found that the optimized meta-atom is robust against experimental variations and conditions such as a non-perfectly collimated incident beam, nanofabrication inaccuracies, and an added substrate. The meta-atoms have been fabricated using two approaches, focused ion beam lithography and an electron beam lithography followed by reactive ion etching, and characterized using white light spectroscopy. To the best of our knowledge, this is the first experimental realization of a machine-learning-based optimization of a magnetic dipole mode at optical frequencies.

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Introduction

Designing Metasurfaces that generate specific optical responses is pivotal for a range of applications, including the enhanced optical nonlinearity, the creation of Fano resonance, and directional light scattering. Significant efforts have already been made to use machine learning to design optical Metasurfaces [1], however, detailed studies on their consisting unit-cells (meta-atoms), their resonant multipolar responses, and internal spatial field distributions are often limited to simple topologies such as spheres or cylinders, which generally support low-order multipolar resonances. If machine learning (ML) can be applied to design meta-atoms with specified high order multipolar resonances, it may facilitate new regimes of light-matter interactions. Recently, our group developed a machine learning based toolbox to design dielectric arbitrary-shape meta-atoms with targeted multipolar resonances within the visible spectrum [2]. By utilizing the multipole expansion theory, our first model, dubbed as the forward prediction model (FPM), efficiently predicts the scattering response of meta-atoms with diverse shapes, whereas the second model, the inverse design model (IDM), designs meta-atoms possessing the desired optical responses at a given operating wavelength as shown in Figure 1. Experimental verification of these meta-atom designs is necessary to validate the theoretical models and reinforce the reliability and applicability of ML in practical nanophotonic applications in the context of Mie-tronics.

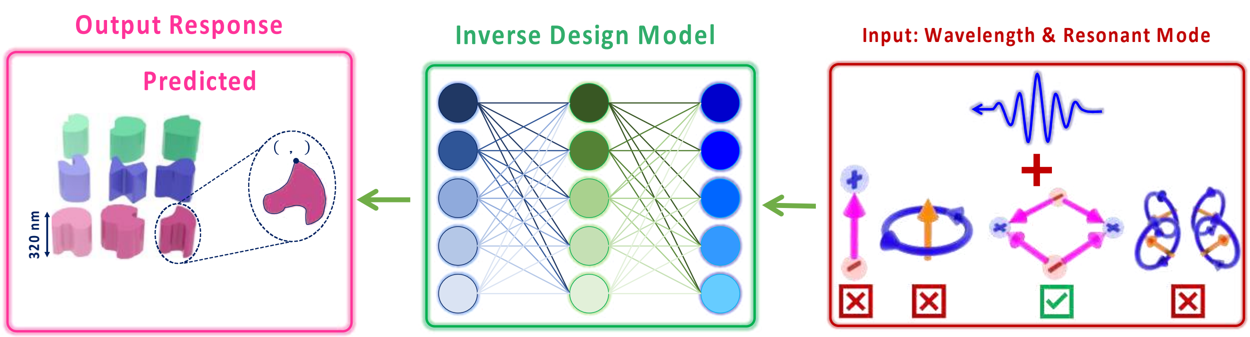

Figure 1. Schematic of inverse design module (IDM) in ML toolbox. The desired multipolar response and the operating wavelength are fed into the IDM which outputs the shape of a 320nm tall Mie resonant scatterer.

Background

The optical response of meta-atom scatterers can be described by a set of electric and magnetic multipoles of different orders. Many meta-atoms with simple shapes, such as cylinders, have multipolar responses dominated by the electric dipole. Achieving a higher order multipolar response typically requires an irregularly shaped meta-atom. Various multipole expansion methods have been employed to design Mie scatterers capable of inducing desired multipole resonances. However, many of these methods only hold for regularly shaped scatterers with dominant electric dipole responses or require inefficient computational solvers. Additionally, designing Mie scatterers for specific multipole responses at a desired wavelength requires brute force optimization processes. The introduction of machine learning into nanostructure design has enabled efficient and effective optimized inverse design for light scattering.

Numerical Predictions

Employing our previously developed IDM, we design a meta-atom possessing an electric dipole (ED) Mie-type resonances at the operating wavelengths of $\lambda_{\mathrm{ED}} = 900$ nm. We first analyze the total scattering cross-sections of the meta-atom isolated in space and on a glass substrate. Due to the inhomogeneous environment (in the case of the substrate) and the differing radiation patterns for the multipoles, the scattering contributions from each individual multipolar response cannot be computed. Instead, the graph for the total scattering cross-section for both cases must be compared to determine if the desired resonance at the operating wavelength is robust against the environment changes as shown in Figure 2(a-b). To further clarify the existence of the desired modes we have also plotted the electric field distribution within the scatterer in the (x-y) plane at the operating wavelength.

Next, the total scattering cross-section was evaluated for a two-dimensional of meta-atoms on a glass substrate. Placing the designed scatterer in a periodic array allows for more accessible experimental characterization of the excited resonant modes. Arranging scatterers in a periodic lattice though, can alter the optical response of structure due to both near- and far-field interactions. To minimize the optical coupling between scatterers, we selected a lattice constant of $p = 1\ \mu m$ for the array which exceeds both the largest dimensions of the meta-atoms and the operational wavelength range. Comparing the calculated field distributions with those obtained from the isolated meta-atom on the glass substrate demonstrates a good agreement in the optical response of both cases at the designed wavelength as demonstrated in Figure 2 (b, d).

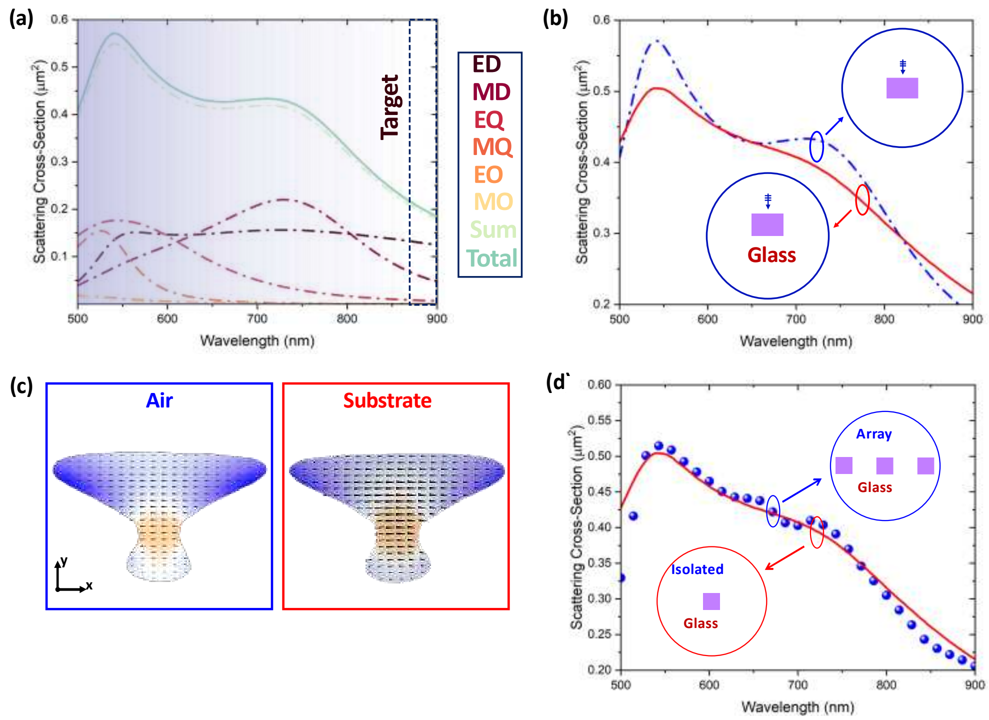

Figure 2. Numerical Simulation Results. (a) The multipolar response of the inversely designed meta-atom in free space is shown. The target wavelength marks the wavelength at which a dominant electric dipole response is desired. (b) The total scattering cross-section is found for the case of the meta-atom in free space and a single meta-atom on a glass substrate. (c) The electric field distributions in the meta-atoms are compared for the two cases described in (b) to further confirm the desired electric dipole response at the target wavelength persists. (d) The total scattering cross-section for the case of a single meta-atom on a glass substrate and a periodic array of meta-atoms on the same substrate is shown.

Experimental Verification

A TiO_2 meta-atom array was fabricated on a glass substrate using electron-beam lithography in combination with inductively coupled plasma etching. We measured the light transmitted through the meta-atoms and divided by that transmitted through the glass. We note that in order ensure the repeatability and validity of our results, we have performed 15 measurements and report the average value as the result. Following the normalized transmittance spectra, the scattering cross-section is calculated. As can be seen from the experimental results shown in Figure 3, the measured scattering response of the fabricated sample closely resembles the theoretical predictions from the developed IDM. Therefore, the suppression/emergence of various scattering modes predicted by the IDM is robust against changes in the dielectric environment and other factors such as periodic configuration.

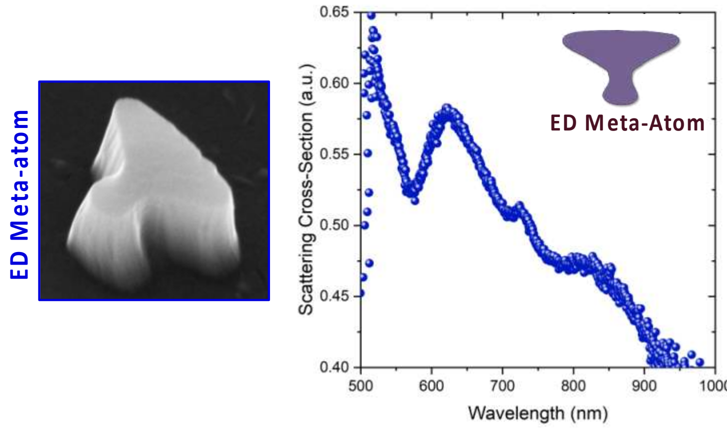

Figure 3. Experimental Results. The total scattering cross-section for a periodic array of meta-atoms on a glass substrate was measured using white light spectroscopy. An SEM image of a fabricated meta-atom is shown above as well.

Discussion

In this work we experimentally validated light scattering predictions from our previously developed ML model for an all-dielectric meta-atom hosting an ED Mie-type resonance. First, the ML model was used to design a meta-atom with a specific ED resonant mode at specific desired operating wavelengths. We explored how the predicted optical response of the designed scatterer alters upon the inclusion of glass substrate, and in a periodic array. The experimental results obtained from the fabricated meta-atoms exhibited good agreement with the predicted results of the developed IDM. Our findings not only serve as the first experimental verification of ML-based Mie-tronics, but also might be a solid step toward the achievement of a fast, versatile, and accurate approach to design meta-atoms with tailored optical response via machine learning and will likely facilitate uncovering new regimes of linear and nonlinear light-matter interaction at the nanoscale as well as a versatile toolkit for nanophotonic design.

References

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