Visualization of angle-dependent plasmonic structural coloration by FDTD-simulated BSDF and ray-tracing rendering

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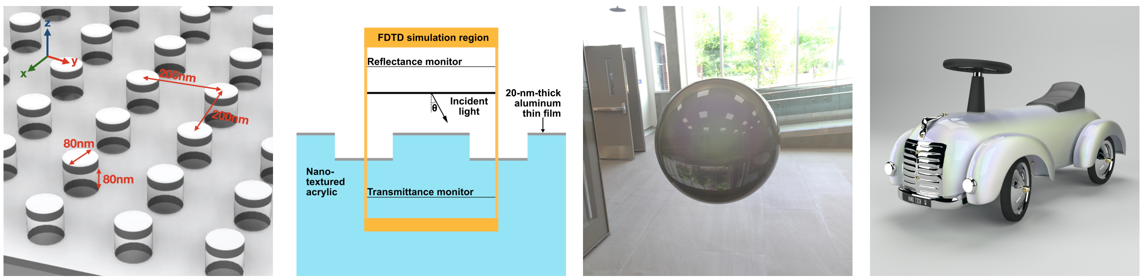

(a) (b) (c) (d)

Figure 1: (a) Schematic diagram of a nanohole and nanodisk array on an acrylic substrate and (b) cross-sectional view of the FDTD simulation region encompassing a single period of the nanostructure. Rendered images of (c) a semi-transparent spherical glass substrate and a (d) pedal car, both coated with a nanohole and nanodisk array layer.

CCS CONCEPTS

• **Plasmonic structural coloration** → **Ray tracing rendering**; • **Nanostructure visualization** → *plasmonic color*; • **FDTD simulation** → ray tracing rendering.

KEYWORDS

plasmonic color generation, FDTD, BSDF, rendering

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1 INTRODUCTION

Plasmonic coloration is the structural coloration that arises from the resonant interaction between visible light and metallic nanostructures, resulting in frequency- and angular-selective scattering and/or absorption [Kristensen et al. 2017]. Structural colouration arising from plasmonic interactions is highly dependent on the configuration and composition of the nanostructure, which include the size, periodicity, and choice of materials [Clausen et al. 2014; Song et al. 2019; Zhu et al. 2017].

Computational visualization of the appearance of metallic nanostructures is not readily achieved, as their visual appearance is governed by electromagnetic interactions on sub-wavelength scales that cannot be captured by traditional ray-tracing rendering methods. Adaption of ray-tracing rendering method to describe metallic nanostructures requires new scattering models that can describe plasmonic effects, including field localization, near-field interference, and surface-bound waves. The ability to generate realistic rendered images of such materials will enable new investigations of their applications in real-world conditions, an important advancement as these materials are currently only produced in labs on small, centimetre-scale substrates.

In this work, we propose to use finite-difference time-domain (FDTD) simulations to generate bidirectional scattering (BSDF) data describing the scattering properties of metallic nanostructures at visible frequencies in a binary material database, which is then used to visualize their appearance by ray-tracing rendering. This approach contrasts with previous ray- and wave-optics models to describe the appearance of Morpho butterfly wings based on FDTD-simulated BRDF models of dielectric nanostructures [Musbach et al. 2013; Okada et al. 2013].

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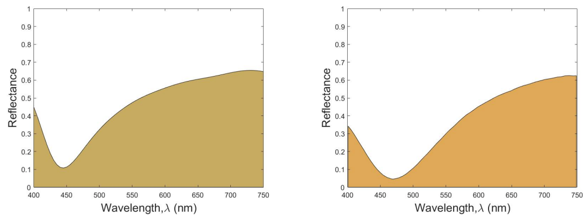

(a) Simulation (b) Experimental

Figure 2: Reflectance over visible frequencies of the nanostructure array at normal incidence (a) calculated by FDTD simulations and (b) measured by reflectance spectroscopy (adapted with permission from [Clausen et al. 2014]).

2 OUR APPROACH

The goal is to develop a rendering pipeline to visualize structural coloration from metallic nanostructures. We examine the configuration of an aluminum nanohole and nanodisk arrays on acrylic (polymethyl methacrylate, PMMA), a well-studied structure with available experimental data on its visual properties [Clausen et al. 2014; Zhu et al. 2017]. We use Lumerical FDTD software to model the time-averaged electromagnetic wave amplitudes transmitted and reflected from the nanostructure array with plane-wave continuous-wave illumination.

The periodic nanoarrays are defined by a textured surface consisting of periodic cylindrical nanopillars on the top surface of an acrylic substrate, where each cylindrical nanopillar has a diameter of 80 nm and a height of 80 nm. The pillars have a periodicity of 200 nm in both lateral directions (x and y) and are arranged in a regular square array. A 20-nm-thick aluminum layer coats the textured surface, covering the top surface of the nanopillars and bottom surface of the substrate, but not the sidewalls of the nanopillars (Figure 1(a)).

A FDTD simulation volume with dimensions of 200 nm $\times$ 200 nm $\times$ 1000 nm captures a single period of the structure, as shown in Figure 1(b). The periodicity of the structure is modelled by periodic boundary conditions along the x- and y- directions. Perfectly matched layers (PMLs) are used along the z-direction, which absorb both transmitted and reflected waves with minimal reflection.

The illumination source is a plane wave that is injected 300 nm above the substrate surface for incidence angles θ varying from 0^o to 85^o and over visible-spectrum wavelengths from 380 nm to 780 nm. The intensity of light reflected from and transmitted through the structure are captured 400 nm above and 300 nm below the substrate surface, respectively. These are converted into reflectance and transmittance values by far-field transformation [Taflove and Hagness 2005]. FDTD simulations yield a BSDF model as a function of wavelength, incidence angle, and azimuthal angle.

To verify the simulation data, we compare the simulated spectral reflectance with experimental measurements. The colors under the curves in Figure 2 represent the reflected color of the nanostructure array derived by simulation and experiment. The simulated color is color matched from the spectral reflectance with the CIE XYZ color system using a standard D65 illuminant. The experimental color was measured from a captured image in a reflection bright field microscope. Figure 2 shows that the simulated data has a minor red-shift and about 26-27% higher reflectance overall compared to experiment data. The simulated color is a darker brown compared to the experimental color. This is attributed to a shifted surface plasmon resonant frequency in the simulations, which do not capture micro- and nano-scale roughness.

We use the material definition language (MDL) in Substance Designer to create a physical-based material model of the nanostructure array. Spectral BSDF is converted into a RGB BSDF using the same color transformation system that system previously described. This data is then converted into a binary data file, .mbsdf, compatible with the Nvidia Iray rendering engine [Corporation 2019; Ford and Roberts 1998].

To highlight the angular-dependent color of the nanostructure, we render the appearance of a spherical glass substrate (Figure 1(c)) and pedal car (Figure 1(d)) coated with the nanostructure array. Figure 1(c) shows that the nanostructure array imparts angular-dependent color on the spherical surface consisting of a pink-colored halo and a gradual color change from a khaki color at the center towards a darker khaki color at the outer edges of the sphere. Figure 1(d) shows similar angular-dependent properties on the pedal car, with noticeable mixtures of pink- and khaki-colored spots on the front body of the car.

3 CONCLUSION AND FUTURE WORK

This work shows the feasibility of using FDTD-simulated BSDF data with ray-tracing rendering to describe structural coloration produced by plasmonic nanostructures. Unlike previous work using FDTD to describe the color of Morpho butterfly wings, this work describes electromagnetic wave interaction with metallic nanostructures to capture complex plasmonic effects that occurring in the near field. Future work will apply this technique to study plasmonic color generation in more complicated structures and under conditions that mimic real-life applications.

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