Multi-scale Computational Visualization of Angle-Dependent and Roughness-Sensitive Plasmonic Structural Coloration

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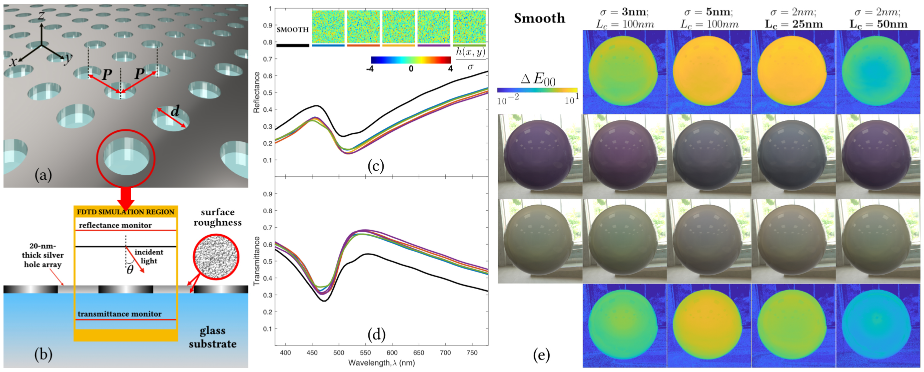

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to preview coated on 3D objects.

Figure 1: (a) Schematic diagram and (b) cross-section view of a unit cell FDTD simulation 20-nm-thick silver nanohole array of coated on glass substrate. (c) Spectral reflectance and (d) transmittance of 20-nm-thick silver nanohole array with a smooth profile and 5 distinct surface roughness profiles (colored lines). (e) Rendered images of smooth and rough silver nanohole arrays coated on spherical substrate in reflectance (second row) and transmittance (third row). The associated color difference, ΔE_{00}, as shown in reflectance (first row) and transmittance (last row). Click the link to preview the plasmonic structural color coated on 3D objects: Link.

CCS CONCEPTS

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

KEYWORDS

plasmonic color generation, FDTD, BSDF, rendering

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1 INTRODUCTION

Structural coloration can be achieved through plasmonic nanostructures tailored on size scales below the wavelength of light. The perceived colors of these structures are highly sensitive to surface geometry and are generally angle- and frequency-dependent [Song et al. 2019]. Fabricated plasmonic nanostructures exhibit roughness which can lead to deviations in its performance compared to those predicted from simulations [Rodríguez-Fernández et al. 2009]. Roughness occurring at nanometer size scales can perturb surface plasmon resonances and, in turn, affect both the far- and near-field electromagnetic field patterns associated with the plasmonic structure[Ge et al. 2018] . Despite considerable progress in coloration technology using plasmonic structures [Lee et al. 2018], there is limited understanding on the impacts of surface roughness on the resulting color produced from plasmonic structures. Physically based rendering (PBR) has enable computational visualization of the visual appearance of complex materials. PBR has been successfully applied to visualize iridescence of Morpho butterfly wings [Musbach et al. 2013], Elaphe snake skin [Dhillon et al. 2014], and soap bubbles [Huang et al. 2020]. State-of-the-art computational visualization cannot be readily applied to investigate structural color from plasmonic nanostructures, as their color is governed by electromagnetic interactions occurring on size scales (10s of nanometers) that cannot be captured by traditional PBR. Adaption

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of PBR to describe metallic nanostructures requires new scattering models which can model subwavelength interactions and incorporate the effects of roughness. The purpose of this work is to explore a multi-scale computational model that leverages electrodynamic simulations and PBR to physically describe the effect of roughness on the structural coloration arising from plasmonic nanostructures.

2 OUR APPROACH

The goal is to investigate the variance of structural color arising from plasmonic nano-structures due to nano-scale roughness. We employ a multi-scale approach that combines finite-difference time domain (FDTD) simulations and PBR, building upon our previous work [Loi and Chau 2020]. We use the well-studied nanohole array configuration in a thin metallic (Ag) film to achieve visible-frequency coloration. We use ANSYS Lumerical FDTD software to model the time-averaged electromagnetic wave amplitudes transmitted and reflected from the nanohole arrays. The silver film is 20 nm thick and coated on a 1000 nm thick glass substrate. The nanohole pattern consists of individual holes of diameter $d = 70nm$ and periodicity $P = 140nm$ in both lateral directions. The configuration is shown in Figure 1 (a).

We define a single volumetric unit-cell in the FDTD simulations with dimension of 200 nm × 200 nm × 1000 nm (Figure 1 (b)). The reflected and transmitted electric field amplitudes are captured by monitors positioned, respectively, 400nm above and 300nm below the substrate. We use periodic boundary conditions along the x- and y- directions and perfectly matched layers (PMLs) along the z-direction. To model nano-scale roughness, the top and bottom surfaces of the silver nanohole array are generated by a surface correlation function [Zhao et al. 1998].

$$\langle H(r)H(r+\delta)\rangle = \sigma^2 e^{-\left(\frac{\delta}{L_c}\right)^2} \tag{1}$$

where $H(r)$ is the surface height at position $r, < \cdots >$ is assembly average, δ is the sampling resolution of the surface, σ is the average root mean square (RMS) of roughness in the vertical direction, and L_c is the correlation length of roughness in plane of the film (x, y). We use randomly generated surface profiles using parameters in listed Table S1 (See the supplemental material).

The nanohole arrays are illuminated by a plane wave injected at 360 nm above the substrate for incident angles, θ, varying from $0^o$to 75^o in steps of 5^o. The incident wavelength is varied over the visible spectrum from 380nm to 780nm in steps of 5nm. The time-averaged reflected and transmitted electric field amplitudes are converted into reflectance and transmittance values through far-field transformation [Taflove and Hagness 2005]. The spectral reflectance and transmittance at normal incident of smooth and rough silver nanohole arrays are shown in Figure 1 (c) and (d), characteristic of a plasmonic resonance. In general, roughness decreases the reflectance of the array across the visible spectrum by about 10% and increases the transmittance above 520 nm by about 15%. These observations are consistent with previous reports of enhanced surface plasmon coupling in rough surfaces, leading to greater conversion of incident light into plasmons and an associated transmission enhancement [Ge et al. 2018].

We employ the material definition language (MDL) in Substance Designer to define a physically based material model of the silver nanohole arrays. We develop spectral BSDF to describe the scattering response of the arrays as a function of wavelength, incident angle and azimuthal angle. We convert the spectral BSDF into a RGB BSDF binary data file (.mbsdf) using CIE XYZ color transformation system with a D65 illuminant [Ford and Roberts 1998]. We use Nvidia Iray rendering engine to render the appearance of the nanohole arrays on a spherical substrate. Figure 1(e) highlights simulated structural colors in reflected and transmitted mode for smooth and rough silver nanohole arrays (with varying vertical and horizontal roughness scale). The nanohole arrays are purple in reflectance and khaki-colored in transmittance, with a slight iridescence apparent from the color change of the sphere at different positions (ie, viewing angles). Discrepancies in the color of the rough arrays compared to that of the smooth array are quantified by the color difference ΔE_{00}. The reflectance is highly sensitive to the vertical roughness parameter σ, as a slight increase from 0 nm to 5 nm (while keeping other parameters constant) changes its hue from purple to grey. Changing the horizontal roughness parameter L_c from 25 nm to 50 nm (while keeping other parameters constant) changes its hue from grey to purple.

3 CONCLUSION AND FUTURE WORK

We demonstrate a novel approach using multiscale FDTD simulations and PBR to study the effect of randomized roughness on structural color as a function of parameters describing surface variations in the horizontal and vertical directions. Future work will examine more complex roughness effects including multi-scale roughness occurring simultaneously at different size scales.

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