Structural colors based on perfect light-absorbed Silicon nanopillars

G J Jin¹, L L Wang¹, J Tan¹ and Y L Meng¹*

¹College of Optical and Electronic Technology, China Jiliang University, Hangzhou, China, 310018

*E-mail: myl@cjlu.edu.cn

Abstract. Perfect light absorption can be realized by many kinds of nanostructures which attributes to various mechanism. In this paper, the reflective property of silicon nanopillar array is studied by simulation. The relation between reflective spectra and the height of silicon nanopillar is discussed. A continuous change of the absorption peak is obtained by adjusting nanopillar’s height. By adjusting the height of the nanopillar, the wavelength of perfect-absorption can be tuned from 400 nm to 800 nm. We also calculated the color coordinate and RGB values. The simulations exhibit a large color rendering area. Our research will be helpful to realize reflective displays and structural color for metrology.

1. Introduction

As colors can provide us many information about the world, they play very important role in our life. In order to obtain more vividly artificial color for application in many fields, lots of ways are proposed. Principally, there are two kinds of mechanisms lied on to realize vivid colors. The first one is due to reflection or scattering of light when lights incident onto the surface of structures. It is a passive manner to render color. The other is due to light emission which needs external power supply. Although color generated by emitting light is the most efficient way to generate bright and pure colors, it cannot be used in passive device.[1] In fact, the mechanism of most colors in nature is lay on the first one. Among these colors, some are generated as a result of light absorption of surface nanostructures, such as colors of flowers, the wings of butter-flies, and some others are generated as results of scattering of nanoparticles, such as sky. Anyway, they are all known as structural colors. In comparison with the color generated by pigments, structural color shows more sustainable and reliable. Up to now, extensive researches on interaction between light and nanostructure have been implemented for the purpose of realizing stable and vivid colors.[2]

Many kinds of nanostructures have the capability to show colors. Metallic nanostructures, one of those nanostructures, are widely used to realize various colors due to its strong resonant plasmonic absorption. The strong resonant plasmonic absorption can realize perfect absorption easily, which leads to a complementary color when the light is reflected by such nanostructures. These strategies also can be used in environment detection due to its sensitivity to environments refractive index, or spread important information secretly such as the Ti-Mg-Ti metasurface [3] provides controllable colors via the environment of the H₂/O₂. In order to manipulate the interaction between light and nanostructure and obtain vivid colors, many nanostructures composed of metal/insulator were also developed. In that nanostructure, the phase and spatial distribution of incident light can be adjusted by
the geometry of metal and insulator nanostructure. At last, the electric field coupling occurs at designed wavelength. Such as Al-Si-Al callenia structure \[4\] gain perfect absorbance in visible light leading to varied colors etc. However, the strong extinction coefficient of metals is an inevitable obstacle for realizing vivid and bright colors.

Due to its mature fabrication process and high refractive index, silicon based nanopillar array attracted more and more attentions in many field, such as solar cells \[5\], SERS \[7\], structural colors. Julien Proust \[1\] gained different colors through changing the cross-section diameters of the nanopillars which help to realized tuned Mie resonance for generating different colors. While such strategies still need complicated processing to fabricate nanorods with different diameters.

Here, we introduce a colored metasurface on the foundation of different heights nanopillar arrays which can be realized only by controlling the etching time. The mechanism of such strategy lies on the effective medium theory which causes perfect absorption of incident light. At last, various complementary color will be generated. In this paper, the reflective properties of silicon nanopillar array is simulated via finite-different time-domain (FDTD) simulations. These nanopillars in the arrays are simulated at the same period and radiuses of the cross-section for the purpose of making sure the height is the only variable factor. And then, the reflective spectrum of the nanopillar arrays with different heights present different absorption wavelengths. By simulation, various colors can be obtained by tuning the heights of nanopillars. Our research will play an important role in the structural color for various industrial applications.

2. Models and Color space
Considering the practical factors, silicon nanopillars array will play an important role in the structural color for various industrial applications. The simulations about silicon nanopillars on Si substrate are completed through FDTD with periodical structures on enough area and enough thickness (much more than the height), and the model has been shown in figure 1. The nanopillars are simulated in the same \(T\) and \(d\), where the \(T\) is the period of the nanopillar array and the \(d\) represents the diameter of the cross-section of the nanopillars.

![Figure 1. The FDTD simulation model](image)

As we all known, the colors the human can see are ascribed to the subjects’ reflectance or emission of the lights into the eyes, which make the whole word colorful. And there are three types cone eyes sensing lights in human eyes. Every kind of cone eye has varied sensitivity to lights at different
wavelengths. All in all, the cone eyes have its sensing peaks in short, middle and long wavelengths, which are corresponding to the three levels of stimulus defined as the tristimulus values. The tristimulus values can be transformed to the three-primary colors to match different color gamut systems and fit different industrial application. The primary colors gain their essential roles with the Grassmanns law laying the foundation of the modern colorimetry. Afterwards, the International Commission on Illumination (CIE,1931)\cite{11} links the reflectance spectrum to multifarious structural colors where the three color-matching functions contribute to transform the spectrum data to tristimulus values calculated via integrating the spectral distribution function in the scope of the visible wavelengths. But the primary colors have different definitions for varied color forming principles.

For the reflectance spectrum, if there is apparent reflectance peak with large-scale high absorbance region in visible light, it is the additive color process that means a way of the colors adding together where the RGB (red, green and blue) is the three-primary colors. So, the RGB three-primary colors are additive model for human eyes getting the adding-together of different light reflected. However, if there is apparent absorbance peak with large-scale high reflectance region in the reflectance spectrum in visible light, it is the subtractive color process that is a way of the color subtracting in the white light where the CMY (cyan, magenta and yellow) is the three-primary colors. Therefore the CMY three-primary colors are subtractive for human eyes getting the lights subtracted some lights. In this paper, all the colors are calculated and confirmed through the original trisimulus values, XYZ and CIE XYZ color space. So, the influence of different color forming principle can be eliminated. Moreover, for convenience, the XYZ values are translated into Adobe RGB values as shown in the later article.

3. Results and discussion
According to our model, the period T of nanopillar array, diameter d of nanopillar are fixed, height of nanopillar array is the only variable parameter to decide the reflectance spectra. In order to gain adequate information about the relationship between the nanopillar height H and the reflectance of nanopillar array, the reflectance changes as H increased is calculated by FDTD simulation. The reflectance spectrum are shown in the figure 2(a), in which the zebra stripe means the wavelength of perfect absorption changes periodically as the height of nanopillar increases from 40 nm to 500 nm. Since the diameter of the nanopillar cross-section and period of nanopillar array keep the same when the height increases, the reason of wavelength modulation is due to effective-medium-theory (EMT).\cite{13}

As the thickness of effective medium changes for the increasing height leading to increase volume fraction in the whole structure, the position of valley of reflectance spectra shifts from 400nm to 650nm. As the previous work has been done, the well-known theory, Bruggeman(BR) approximations\cite{14,15} is always used to explain the EMT. The BR approximations take all the constitutions into consideration and calculate the effective dielectric constant of the mixture of air and silicon here. As the height of the nanopillars changes, the volume fraction of silicon in the mixture and the structure and morphology are all changed.

In the zebra stripe picture, the dark blue region means a low reflectance of the incident light. Conversely, brighter-color region indicates a higher reflectance where the maximum is about 0.357(35.7\%) in the range of this case. As the height increases to 400nm, there are three absorption valleys. That means the more perfect absorbance valley with the higher nanopillar. For examples, there are two valleys for nanopillar with height of 200nm in wavelength range from 400nm to 800nm. However, there are three valleys for height of 300nm and four valleys for height of 500nm. It accordance with the thin film interference when the thickness of effective medium increases. Furthermore, such modulation is periodic.
In figure 2 (b), the more detailed reflectance spectra with different nanopillar height are compared. Different absorbance peaks leads to vital influence to the coloration. The color coordinate of those reflective spectra is calculated by three color-matching functions, \( x \), \( y \), and \( z \), which were established from experiments on a standard observer by 1931 CIE \( x,y \) as mentioned above. In order to gain a series of colors, the reflectance spectrum of different heights and their corresponding colors listed in the figure 2(b) are calculated through color-matching functions. Obviously, the colors listed beside the \( H \) row varied continuous when the height of the nanopillar \( H \) increases. The valley of reflectance spectra firstly appears at the wavelength of 400nm when the height is 40nm, and then, the zero-valleys appears in 492nm, 628nm, 749nm and 898nm when the \( H \) is 60nm, 80nm, 100nm and 120nm respectively. As the \( H \) increases, the positions of peaks and valleys shift to red. The number of valley also increases which indicates multi-absorption occurs.

As mentioned above, the colors human can see result from the combining work of the spectrum and the sensitivity of the eye cone cells. The spectrum are matched with the tristimulus values via the three-matching functions, \( \bar{x}(\lambda), \bar{y}(\lambda) \) and \( \bar{z}(\lambda) \). After obtaining the tristimulus values, \( X,Y \) and \( Z \), in fact, we have already got the corresponding colors of the spectrum which can be ascertained in the CIE XYZ color space based on three normalized values, \( x, y \) and \( z \). The \( x \), \( y \) and \( z \) are calculated via the tristimulus values with \( x=X/(X+Y+Z), \ y=Y/(X+Y+Z) \) and \( z=Z/(X+Y+Z) \). For widely used CIE RGB color space, it tends to be similar. There are also RGB three-matching functions, \( \bar{r}(\lambda), \bar{g}(\lambda) \) and \( \bar{b}(\lambda) \), the RGB tristimulus values \( R, G \) and \( B \), and three normalized values. It is a \( 3 \times 3 \) transformation matrix that transform the XYZ into RGB with \( [R, G, B]=M[X,Y,Z] \).

The RGB values and the colors of every height nanopillar involved are presented in the figure 3. In the figure, the curves are fitting with the original scatter diagrams and the red curve is about the R values calculated from XYZ, the same for G and B. The oscillation RGB value curves echo the valleys moving in the figure 2 (b). As the \( H \) increases, the valley moves to the red part of the spectra and new valley appears in the blue part. Afterwards, we mark the colors in the CIE XYZ color space. So, there is a color region circled by the peripheral points as shown in figure 4 based on the chromaticity coordinate (\( x, y \)). The color region has embraced a big range of colors, which means plenty of
structural colors can be realized through the $H$ changing. Also, in the color region, the similarity between colors takes place when the heights are too close numerically or the heights changes periodically. For example, use $H(x, y)$ to represent the chromaticity coordinate $(x, y)$ of different $H$ in CIE XYZ color space. The 40 nm $(0.4076, 0.4140)$ and 50 nm $(0.4834, 0.4357)$ are really two close points in the color space, which leads to similar coloration for the 40nm and 50nm height nanostructures. The 140 nm $(0.3831, 0.4422)$ and 280 nm $(0.3845, 0.4592)$ are also really close to each other for the $x$ and $y$ in the color space, which also leads to similarity in coloration. Just like the period of coloration mentioned above, the 140nm and 280nm showing similar colors can be owing to the period, but the certain period of the coloration can be gained through statistic analysis based on mass of data which needs a further research.

4. Conclusions
In conclusion, full colors are obtained by adjusting the perfect absorption wavelength of nanopillar array. The realization of perfect absorption lied on effective medium theory which results in the perfect absorption wavelength red shift when the height of silicon nanopillar array increased. The tristimulus values of these complementary colors on 1931 CIE $x,y$ diagram indicates a wide-range color can be generated. Moreover, the colors tend to show periodically as the nanopillar height $H$ changes. Our research also provides a new simple way to realize vivid structural color only by adjusting nanopillar’s height. The results will be helpful to be applied in solar cells and filters.

Acknowledgments
Thanks for the supports of National Key Research and Development Program (No. 2017YFB0403501), Zhejiang Provincial Natural Science Foundation (No. LQ15F040004), the Open Fund of the State Key Laboratory of Integrated Optoelectronics (No. IOSKL2015KF28) and the Talent Development Project in Photoelectric Detection of Top Priority Construction Subject of Instrument Science and Technology of Zhejiang Province (No. JL150540).
References

[1] Julien P, Frederic B, Bruno G, Igor O and Nicolas B 2016 All-dielectric colored metasurfaces with silicon Mie resonators J. ACS. Nano 10 7761-67

[2] Shang S, Zhenxing Z, Chen Z, Yisheng G, Zonghui D, Shumin X and Qinghai S 2017 All-dielectric full-color printing with TiO2 surface J. ACS Nano 11 4445-52

[3] Xiaoyang D, Simon K, Na L 2017 Dynamic plasmonic color display 2017 J. Nature Communication 8 14606 1-9

[4] Seyed S.M, Ting S and Junpeng G 2016 Zeroth order Fabry-Perot resonance enabled ultra-thin perfect light absorber using percolation aluminum and silicon nanofilms J. OPTICAL MATERIALS EXPRESS 6 1032-42

[5] Hemant K.R, Anand G, Sreekumaran N and Seeram R 2011 Anti-reflective coatings: A critical, in-depth review J. Energy Environ. Sci. 4 3779-3804

[6] Chih-Hung S, Peng J and Bin J 2008 Broadband moth-eye antireflection coatings on silicon J. APPLIED PHYSICS LETTERS 92 061112

[7] L D, S Y 2016 Effect of nanogap curvature on SERS: a finite-difference time-domain study J. Journal of Physical Chemistry C 120 20642-650

[8] Zilei W, Shanglong P Yuxiang W Tianfeng Q, Qiming L, Deyan H and Guozhong C 2017 High-performance Si/organic hybrid solar cells using a novel cone-shaped Si nanoholes structures and back surface passivation layer J. Nano energy 41 519-26

[9] Shang S, Wenhong Y, Chen Z, Jixiang J, Yisheng G, Xiaoyi Y, Qinghai S and Shumin X 2018 Real-time tunable colors from microfluidic reconfigurable all-dielectric metasurfaces J. ACS Nano

[10] Alessia I, Maria J, Cristiano D, Antonio A.L, Pietro A, Barbara F, Rosaria A.P, Nicola C, and Sebastiano T et.al 2017 Light emitting silicon nanowires obtained by metal-assisted chemical etching J. TOP Science

[11] T S, F I, J G 1932 The C.I.E colorimetric standards and their use J. Transactions of Optical Society 33 73-133

[12] Huge S.F, Michael H.B, Henry H 1996 How the CIE1931 color-matching functions were derived from Wright-Guide data J.COLOUR research and application 22 11-23

[13] Vijaya K.G and Shreepad K 2017 Effective medium theory based analytical models for the potential and field distributions in arrays of nanoscale junctions J. JOURNAL OF APPLIED PHYSICS 122 024502

[14] Han W, Xianglei L, Liping W and Zhuomin Z 2013 Anisotropic optical properties of silicon nanowires arrays based on the effective medium approximation J. International Journal of Thermal Sciences 65 62-69

[15] M K , M B and B B 2007 Bruggeman effective medium approach for modelling optical properties of porous silicon: comparison with experiment J. phys. stat. sol. 4 1986-90

[16] Henrie J, Kellis S, Schultz S and Hawkins A 2004 Electronic color charts for dielectric films on silicon J. Opt. Express 12 1464-69