メタサーフェイス設計のための微細周期溝構造の近接場位相応答解析
Near-field Phase Analysis of Periodic Microgroove Structure for Metasurface Design based on FDTD Simulation

東京大学　○管一兆　増井周造　門屋祥太郎　道畑正岐　高橋哲，東京農工大学　岩見健太郎，宇都宮大学　稲秀樹
The University of Tokyo, ○Yizhao Guan, Shuzo Masui, Shotaro Kadoya, Masaki Michihata, Satoru Takahashi,
Tokyo University of Agriculture and Technology, Kentaro Iwami, Utsunomiya University, Hideki Ina

1. Introduction

Microstructures are widely used in the manufacture of functional surfaces. A simple and effective design of microstructures is the periodic microgroove structure. This structure has been well-known as gratings. Gratings are well understood in the diffraction regime, where the terms of diffraction orders are used when the wavelength is much smaller than the grating period, and the deep-subwavelength regime, where the effective medium theory can be applied when the wavelength is much larger than the grating period. Between these two regimes, the periodic microgroove structure has distinct features such as high reflectance and high transmittance. When the substrate is neglected for simplicity, the periodic bars with a size of the middle regime are also called high-contrast gratings (HCGs) [1]. Theoretical analysis based on waveguide theory has been conducted to explain the high reflectivity and high transmission phenomenon of HCGs [2].

Optical metasurfaces can be designed based on manipulation of the meta-atom (a unit cell of the metasurface), and the phase retardance effect of the designed structure is determined by the combination of meta-atoms. Previous researchers have successfully designed microscale planar focusing reflectors and lenses with a focal length of ten micrometers with HCGs [3]. The microgroove structure and its applications are illustrated in figure 1.

However, this complex behavior of periodic microgrooves or HCGs involves many parameters. The polarization and wavelength of illumination and structure features such as period, filling factor, and bar height affect the phase retardance. The period structure response can be understood by building a library with numerical methods with parameter scans. The features of periodic microgrooves become more complicated in the design of metasurfaces for phase control. In this work, a design strategy by combining microgrooves with only filing factor difference while fixing the period and bar height is proposed. The simulation for periodic microgroove structures and the combination of different filling factor units is conducted based on the Finite-Difference Time-Domain (FDTD) method to study how the variance in the mixture of periodic structures varies the near-field phase retardance.

2. Phase retardance of periodic microgrooves structure

Firstly, the periodic model is shown in figure 2(a). The simulation is supposed to be one of the design processes for metasurfaces with amorphous silicon working at the near-infrared region. The substrate is taken as silicon as well. Light incidents from the substrate, and the transmission phenomenon is studied. Horizontally the periodic boundary condition (PBC) is set while the absorption boundary condition (ABC) is set vertically. The wavelength is fixed at 900 nm and the period is fixed at 400 nm. In figure 2 (b), the power distribution at filling factor 0.5, height 400 nm is shown while the power is normalized by the incidence. The resonance induced by the layer of microgrooves can be observed.

By scanning the height and filling factor of the bar, we can obtain the phase retardance and transmittance for TM waves as shown in figure 3. The design of an optical meta-atom requires a 2π change of phase retardance. The bar height should be constant for easy fabrication. According to the simulation, it was found in figure 4 that at 440 nm height, a stable transmission can be obtained while the phase retardance can be tuned by changing only the filling factor, under TM illumination.

3. Phase retardance of periodic microgrooves structure combination

Next, the effect of the mixture of periodic units is going to be investigated. One unit is composed of the same microgroove structures and the unit length is the number of periods times the length of one period. Since the far-field phase of optical metasurfaces can be determined by the convolution of the near-field complex amplitude and point spread function of the imaging system, the near-field phase distribution is investigated in detail. In figure 5, the near-field phase distribution is shown for periodic units with filling factor of 0.5 and 0.1. The combinations of these two units are analysed. The center periodic unit has filling factor of 0.5 and the filling factor of surrounding periodic unit is 0.1. To investigate effects of the number of periods only at the center, the period number of surroundings units is set to be large enough. The center period number affects the distribution shape. It is found that the center distribution are almost the same compared to periodic case for 7 period number unit in figure 6. When the unit length is over 2800 nm, about 3 times of the wavelength, the surroundings doesn't affect the nearfield phase of center period unit.

Finally, the effect of period number is investigated for less period number as shown in figure 7. When there are only 1 and 2 period structures, the phase at center area has been effected by surroundings. This result suggests that the phase adjustment can also be conducted through control of period number in every unit.

4. Conclusion

The results obtained by FDTD analysis in this paper are summarized as follows.

Firstly, to find a proper bar height for optical meta-atom, the phase retardance and transmission are obtained for periodic microgroove structure with the periodicity of 400 nm under near-infrared illumination of 900 nm. Based on this data, the bar height is determined to be 440 nm for silicon substrate so that transmittance is relatively stable while the phase retardance can be changed over 2π by changing the filling factor.

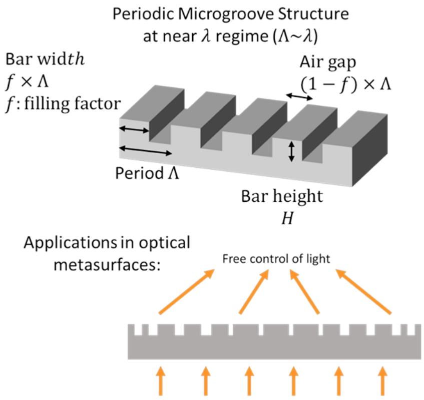

Figure 1: Near-wavelength periodic microgroove structure is the fundamental design of functional surfaces, which has applications in optical metasurfaces such as metalens and so on.

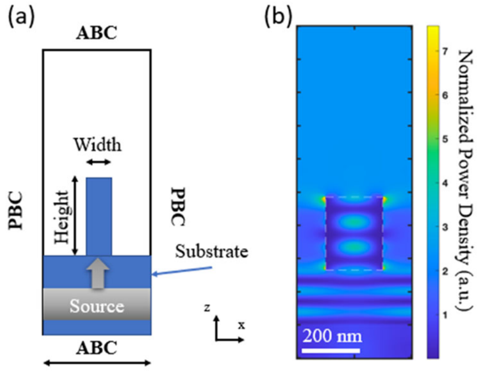

Figure 2: (a) Set up for FDTD analysis of periodic microgroove strcutures. (b) Power density distribution normalized to incidence.

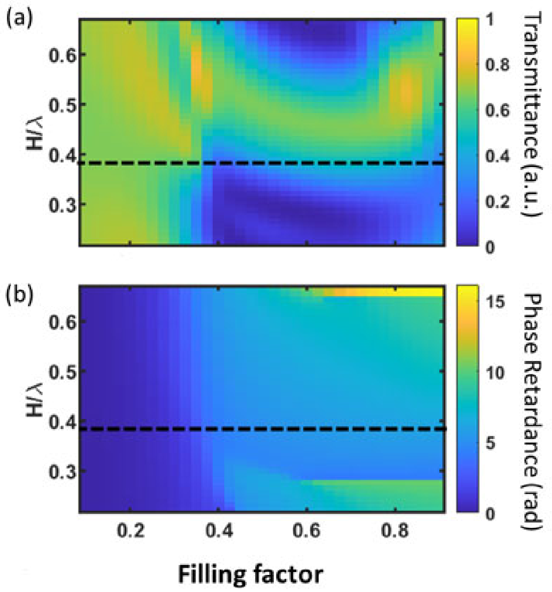

Figure 3: Simulation results when scanning the bar height (normalized to wavelength) and filling factor for (a) transmittance and (b) phase retardance for TM case. At the dashed line bar height, a stable transmission value at high level is obtianed while the phase retardance can vary over 2π (6.28 rad).

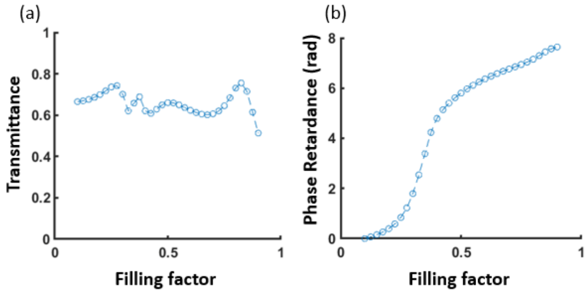

Figure 4: When bar height is 440 nm, (a) the transmittance varies between 0.6 and 0.8 with filling factor variance while (b) the phase retardance can vary over 2π comparing to the case of filling factor 0.1.

Secondly, the near-field phase is investigated in detail. The design of phase variance can be achieved by the combination of period units. It is found that the surrounding effects can be neglected when the unit length is over 3 times the wavelength. But the phase of a single structure is affected by its surroundings when the period number is small in the unit.

Finally, the phase retardance adjustment can be achieved by changing the period number, providing a flexible design strategy for optical metasurfaces.

Acknowledgment

This work was supported by JSPS KAKENHI Grant Numbers JP19H02036.

6. References

[1] C. J. Chang-Hasnain and W. Yang, “High-contrast gratings for integrated optoelectronics,” *Adv. Opt. Photonics*, vol. 4, no. 3, p. 379, 2012, doi: 10.1364/aop.4.000379.

[2] V. Karagodsky, F. G. Sedgwick, and C. J. Chang-Hasnain, “Theoretical analysis of subwavelength high contrast grating reflectors,” *Opt. Express*, vol. 18, no. 16, p. 16973, 2010, doi: 10.1364/oe.18.016973.

[3] F. Lu, F. G. Sedgwick, V. Karagodsky, C. Chase, and C. J. Chang-Hasnain, “Planar high-numerical-aperture low-loss focusing reflectors and lenses using subwavelength high contrast gratings,” *Opt. Express*, vol. 18, no. 12, p. 12606, 2010, doi: 10.1364/oe.18.012606.

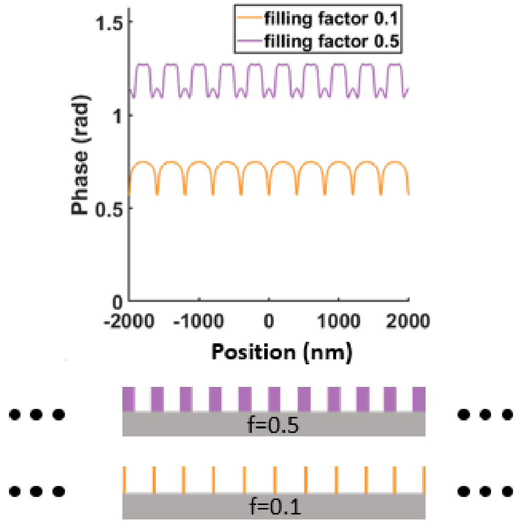

Figure 5: The near-field phase distribution 20 nm above the microgrooves top surface is shown for periodic units with filling factor of 0.5 and 0.1, when the height is fixed at 440 nm. The bar induces phase delay because of high refractive index.

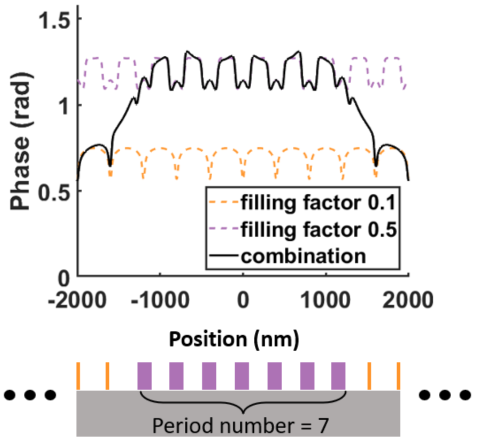

Figure 6: The near-field phase distribution of periodic units combination, of which the center filling factor is fixed at 0.5 while the surrounding filling factor is 0.1. When center period number is 7, the center phase distribution can be considered unaffected by surroundings.

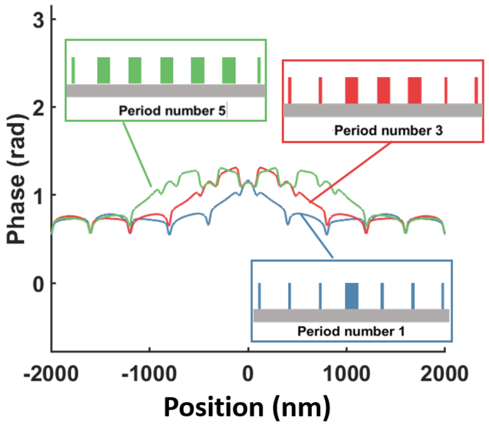

Figure 7: The near-field phase distribution of periodic units combination when center period number is small. The distribution is shown for surrounding filling factor is 0.1 while center filling factor is 0.5, and the number of center period is 1,3 and 5.