Suppression of reflection peaks caused by moth-eye-type nanostructures for antireflection applications studied by using FDTD simulation

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ABSTRACT
Various nanostructures have been adopted for anti-reflection coating due to the graded refractive index. The interference between the two interfaces may sometimes cause an oscillating reflectance spectrum under certain conditions. The anti-reflection performances of a few nanostructure arrays were investigated using the finite-difference time domain (FDTD) simulation method. The study showed that the appropriate modulation of the height of nanostructures is a very effective method for suppressing the reflection peaks and flattening the reflectance spectrum.

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1. Introduction
Efficient anti-reflection structures are very important in various applications, such as solar cells, photodetectors, and display technology [1,2], where the reflection losses should be minimized. Several optical structures, such as dielectric multi-layer coating and index-matching layer, have been used for antireflection purpose. Adopting periodic nanostructures mimicking moth eyes is another efficient anti-reflection method because of such nanostructures' grading refractive index [1–5]. In this case, the nanostructures in the coating layer are generally tapered, and the air fraction decreases in the coating toward the substrate. There are several ways to form subwavelength nanostructures on a flat substrate: through subwavelength surfaces holographically recorded and etched into silicon wafers [6], reactive ion etching [4], wet etching [7], the templating technique [8], various lithography technologies [8], etc.

In many moth–eye nanostructure cases, successive local maxima and minima are observed from the reflectance spectrum [8–11]. Their appearance is attributed to the thin-film interference and is known to be sensitive to the pitch of the array [9]. The oscillating reflectance may be troublesome because it will cause coloration of the reflected light toward specific viewing directions. Conical shapes with two different heights were adopted by Yang et al. [11] to suppress the reflection peaks. In the present study, another scheme was proposed to suppress the oscillating reflectance. The effect of the height modulation of several nanostructures on the reflectance spectrum was investigated using the FDTD (finite-difference time domain) method. It was found that the sinusoidal modulation of the height is very effective in suppressing the reflection peaks and flattening the reflectance spectrum.

2. Simulation
A commercial software (RSoft, ver.06-1, Synopsis Co.) was used to carry out FDTD simulation. Figure 1 shows a schematic diagram showing the 2D (two-dimensional) simulation of the moth–eye structure. Plane waves in the visible range are generated from the plane wave source and are normally incident on the nanostructure made from SiO2 (refractive index: ~1.46). Both the reflected and transmitted waves were monitored to calculate the reflectance and the transmittance. Two plane waves with TE and TM polarization components were used for the simulation, and the average value obtained from these two components was used to calculate the reflectance.

Figure 2 shows the 2D moth–eye type nanostructure designed for anti-reflection purpose. It shows the relationship between the width and the height of this structure. The curvature of the 2D nanostructure was designed...
according to the following equation:

\[ w(z) = w_0 \sqrt{1 - \frac{z^2}{h^2} + \frac{w_0^2}{h^2}}, \]

where width \( w \) at height \( z \) was determined at a fixed value of \( w_0 = 150 \text{ nm} \) and total height \( h \). The \( h \) was changed from 600 to 1000 nm. In this case, the bottom width was \( w_0 \sqrt{1 + \frac{w_0^2}{h^2}} \), and the width at the top of the nanostructures was \( \frac{w_0^2}{h} \). Similar parabolic shapes were adopted in other simulation studies [8,12]. In one simulation run, total height \( h \) was fixed to a certain value. In the second run, the height was modulated sinusoidally according to the equation \( h = h_0 + 100 \cos(2\pi x/p) \), where \( h_0 \) is the average height, \( x \) is the coordinate along the horizontal direction, and \( p \) is the pitch.

For the 3D (three-dimensional) simulation, three shapes were chosen, as shown in Figure 3, which were arrayed in a hexagonal lattice. The first shape was a cone, where the bottom radius was fixed to 100 nm and the height was changed from 700 to 1000 nm in 100 nm increments. The pitch of the array was 300 nm. The second structure had a modified conical shape where cross-sectional width \( w \) was changed according to the function of \( \sqrt{z} \). The base radius was fixed at 210 nm, and the height was changed from 700 to 1000 nm in 100 nm increments. The pitch of the array was 450 nm. The last shape was a combination of a cone and a sphere, which was recently realized by polymer self-assembly [13]. The dimensions and pitch of this array were exactly the same as those of the first one (i.e. the cone array). The radius of the sphere was 50 nm. Recent experimental studies showed that various nanostructures can be realized, and their physical parameters can be controlled in sophisticated experiment procedures [14,15]. The heights of these three arrays were also modulated sinusoidally according to \( h = h_0 + 100 \cos(2\pi x/p) \), where the physical meaning of each parameter is the same as that in the 2D simulation.

3. Results and discussion

Figure 4 shows the wavelength-dependent reflectance of the SiO₂ substrate without any nanostructure. It shows 3.5–3.7% reflectance in the visible range, which is consistent with the estimation based on the Fresnel equations. The wavelength dependence of the reflectance was related to the dispersion of the refractive index of SiO₂.

Figure 5 shows the wavelength-dependent reflectance of the SiO₂ substrate on which the 2D nanostructure (shown in Figure 2) was formed as a function of either the pitch or the height. In the figures, ‘p0.2’ and ‘h0.6’ indicate a ‘200 nm pitch’ and a ‘600 nm height,’ respectively, for example. ‘cos’ denotes the reflectance for the case of the sinusoidal modulation of the height. Figure 5(a)
shows the reflectance as a function of the pitch at a fixed height of 1000 nm. The reflectance shows an oscillating behavior in the visible region, and the average reflectance decreases as the pitch increases from 200 to 350 nm. Similar successive maxima and minima in the reflectance spectrum are frequently observed from the moth-eye anti-reflection coatings [8–11]. The dependence of the reflectance maxima on the pitch is related to the interference by the two interfaces of the moth-eye layer [9]. In addition, the reflectance decreases as the pitch increases. This indicates that the effective refractive index, which depends on the pitch and can be calculated using the effective medium theory, becomes more gradual as the pitch increases. Figure 5(b) shows the wavelength-dependent reflectance simulated as a function of the height at a fixed pitch of 300 nm. The general trend noticed from this result is that the average reflectance becomes lower as the height increases. The data for ‘cos’ denote the case of the sinusoidal modulation of the height. At a fixed height, the reflectance exhibits successive maxima and minima. This significant oscillation of the reflectance is suppressed under the condition of height modulation. That is, the sinusoidal modulation of the height superposes the reflection peaks caused by various heights, and thus, the reflectance becomes nearly independent of the wavelength. The average reflectance under height modulation is close to the mean maximum and minimum values obtained without any modulation.
Figure 5. (Color online) Wavelength dependence of the reflectance (a) as a function of the pitch at a fixed height of 1000 nm, and (b) as a function of the height at a fixed pitch of 300 nm. ‘p0.2’ and ‘h0.6’ indicate a ‘200 nm pitch’ and a ‘600 nm height,’ respectively. ‘cos’ denotes the case of the sinusoidal modulation of the height.

Figure 6. (Color online) Wavelength dependence of the reflectance of (a) the cone nanostructure, (b) the modified conical nanostructure, and (c) the cone–sphere nanostructure.
Figure 7. (Color online) Schematic figure of the height-modulated 3D nanostructures.

Figure 8. (Color online) Wavelength dependence of the reflectance of (a) the cone nanostructure, (b) the modified conical nanostructure, and (c) the cone–sphere nanostructure together with the results of the height-modulated structure indicated as ‘cos.’
This result shows that the height modulation of nanostructures is a powerful method of suppressing the wavelength dependence of the reflectance of moth-eye-type anti-reflection coatings.

Figure 6 shows the reflectance for the 3D nanostructures placed in a hexagonal array with a fixed pitch of 300 nm. Figure 6(a) exhibits the wavelength dependence of the reflectance of the cone structures at four heights. The reflectance increased with the increase in wavelength, although the oscillating behavior persisted. Figure 6(b) shows that the reflectance of the modified conical structure increased monotonically with the increase in wavelength. In contrast, the reflectance of the cone–sphere structure shown in Figure 6(c) displayed a significant oscillating behavior in the visible range. These differences may be understood by noting the structural differences among the three cases. In contrast to the cone or modified conical structure, the cone–sphere structure was characterized by the sphere layer that faced the incident light. The existence of the sphere layer caused a relatively sudden change in the refractive index, which in turn enhanced the thin-film interference, resulting in the oscillating behavior, as shown in Figure 6(c). On the other hand, the clear distinction between the air and the nanostructures was smeared out in the case of the cone and modified conical structures. Especially, the volume ratio of air of the modified conical structure was the highest among the three structures, which induced nearly no interference pattern in the reflectance curve, as shown in Figure 6(b). This gradual change in the effective refractive index at the interface is a favorable condition for low reflectance; indeed, the reflectance of the modified conical structure was the lowest among the three structures. This shows that a smaller refractive index gradient is important for achieving lower reflectance.

Cone and modified conical structures with sharp tips, however, look unstable to external pressure. This mechanical instability may be compensated for by the cone–sphere structure. The significant reflectance oscillation, which is a shortcoming of the cone–sphere structure,

![Figure 9](image-url)

**Figure 9.** (Color online) Wavelength dependence of the reflectance of the cone–sphere nanostructure for the two incidence angles: 15° [(a) without and (b) with cosine modulation] and 30° [(a) without and (b) with cosine modulation].
structure, can be suppressed by modifying the height sinusoidally. Figure 7 shows a schematic figure of the height-modulated 3D nanostructures. Figure 8 exhibits the effect of the height modulation on the reflectance. The most interesting results can be seen in Figure 8(c), where the successive maxima and minima of the reflectance were suppressed by the sinusoidal modulation of the height. Height modulation superposes and averages the different reflection peaks caused by the different heights, and may also reduce the gradient of the refractive index.

As the oscillating reflectance may cause coloration of the reflected light along a certain viewing angle, suppression of the oscillating reflectance in terms of height modulation may be a useful method of preventing the formation of reflection peaks. The additional simulation that was carried out under the condition of oblique incidence showed that the sinusoidal height modulation significantly suppressed the reflectance oscillation over a wide incidence angle range (from 15° to 45°). Figure 9 shows that the cosine modulation of the height was helpful in suppressing the reflectance oscillation for the two incidence angles of 15° and 30°.

Finally, it should be pointed out that other types of height modulation can also be adopted for suppressing the oscillating reflectance of nanostructures, because a gradual change in the refractive index can be reached by adjusting the relative ratio between the air and the material comprising the anti-reflection layer in various ways. Considering that a gradual change in the volume ratio between the air and the material is important, sinusoidal or sawtooth modulation is more favorable for this purpose than abrupt shape change, such as into a square-type nanostructure.

4. Conclusion

The anti-reflection performances of a few nanostructures, including parabolic, cone, modified conical, and cone–sphere nanostructures, were investigated using the FDTD simulation technique. All the nanostructures exhibited lower reflectance values compared to the bare SiO₂ substrate. The reflectance displayed successive maxima and minima on the reflectance spectrum under certain conditions, which were attributed to the thin-film interference. The sinusoidal modulation of the height of the nanostructures successfully suppressed the reflection peaks and flattened the reflectance spectrum.

Disclosure statement

No potential conflict of interest was reported by the authors.

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