Different theories of analysis and calculation for the reflection efficiency of antireflective nanostructures

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We attempt to analyze different theories for the calculation of antireflective nanostructures. How to choose an appropriate theory and the reason is considered in given conditions. Based on our analysis, effective medium theory (EMT) is unsuitable for nanostructures with a dimension (period) much smaller than the incident wavelength, as higher order diffraction waves other than the zeroth order diffraction propagate here. Rigorous coupled wave analysis (RCWA) can only be used in rigorously periodic conditions because the boundary conditions must be periodic, no matter the dimension of period. Finite element method (FEM) can be used in any conditions but with an excessive computation consumption.

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1. Introduction

Antireflective nanostructures have attracted enormous attention recently because they can dramatically suppress the reflection losses and increase transmission of light at the interface simultaneously over a large range of wavelength and a large field of view [1], which are crucial to the performance of optical and electro-optical devices. For example, the antireflective nanostructures on solar cells can improve the efficiency of them [2,3], and in flat panel display or detector applications, antireflective surfaces are usually employed to increase transmission and eliminate ghost images or veilglare caused by reflection from the optical surfaces, promoting the performance of the devices [4].

In order to design appropriate nanostructures before fabrication, different theories have been proposed for analyzing and calculating the reflective characteristics of antireflective nanostructures. For example, effective medium theory (EMT) approximates the antireflective surface to a stack of homogenous thin film with the effective gradient indices of refraction [5]. Rigorous coupled wave analysis (RCWA) has been commonly applied to yield accurate Maxwell's equations to calculate the reflective efficiency [6]. Some other methods such as the finite element method (FEM) and the finite-difference time-domain (FDTD) method provide numerical calculations to obtain the reflected optical power of the structures [7].

These theories contribute a lot to analysis, design and optimization of antireflective nanostructures. However, there are also limitations and applicable conditions for each theory. Until now, little research has been done on the comparison of these theories or how to choose an appropriate theory in a given condition. Therefore, in this paper we provide some effective analysis and clarify the reason why some theories are suitable while others are not, which is significant for researchers to effectively design and analyze a nanostructure with high quality under different conditions, besides, give a guide to comprehend those theories.

2. Theory heading

The schematic illustration of an antireflective nanostructure is shown in Fig. 1. Λ and h represent the period and groove depth, n_0 and n_g are the refractive indices of the incident medium and substrate medium, respectively.

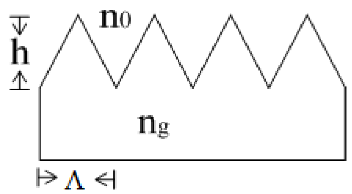

Fig. 1. The schematic illustration of a nanostructure.

2.1 Effective medium theory (EMT)

When the period or irregularity of antireflective surface nanostructure is much smaller than the incident wavelength, EMT is available to analyze and calculate the reflective characteristics [8, 9, 10]. A nanostructure surface can be approximated as a set of multiple layers of the ‘‘effective medium’’ having refractive indices (RI) in the limit of the substrate and ambient. The effective RI (n) of the ‘‘effective medium’’ can be approximately obtained from the filling factor (f) of the individual rough layers. The effective RI (n) of the mixture will be given by

$$\frac{n^2-n_1^2}{n^2+2n_1^2}=(1-f_1)\frac{n_2^2-n_1^2}{n_2^2+2n_1^2} \quad (1)$$

n_1 and n_2 are the RIs of the substrate and ambient, respectively. The antireflective nanostructure can be approximated to a number of lamellar grating layers with different filling factors as shown in Fig. 1. As a result, the nanostructure can be regarded as massive pieces of homogenous layers with effective gradient RI, moreover, the incident and substrate medium are supposed to be homogeneous. Then the reflectances can be analysed using thin-film optics theory.

2.2 Rigorous coupled-wave analysis (RCWA)

To analyze and calculate the reflective characteristics of antireflective nanostructures, RCWA is widely used for obtaining the exact solution of Maxwell’s equations [11, 12].

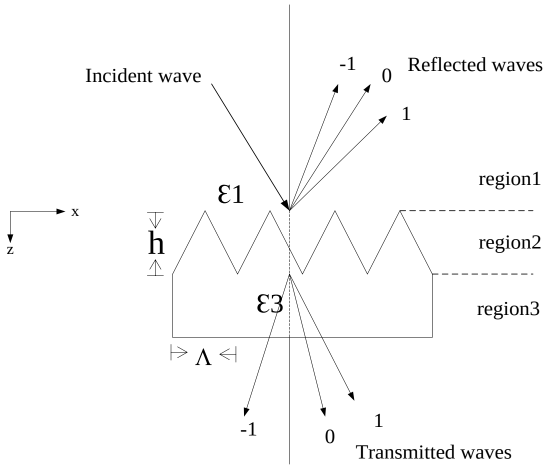

Fig. 2. The geometry for reflection and transmission of a nanostructure.

As is shown in Fig. 2, the whole structure can be further divided into three regions: incident (region 1), grating (region 2), and exit region (region 3).

The boundary between the ε_1 (relative permittivity of region 1) dielectric and the ε_3 (relative permittivity of region 3) dielectric in region 2 is givenby

$$z = F(x) = F(x+\Lambda) \quad (2)$$

Here, Λ and h represent the period and groove depth, z and x are the coordinates of the structure, we choose TE mode for simplicity.The total electric field in region 1 is the sum of the incidentand the backward-traveling wave. The normalized totalelectric field in region 1 can be expressed as

$$E_1 = exp(-j\vec{k}_1\cdot\vec{r}) + \sum_{i=-\infty}^{\infty} R_i \exp(-j\vec{k}_{1i}\cdot\vec{r}) \quad (3)$$

Where k_1 is the incident-field wave vector ofmagnitude, R_i is thenormalized amplitude of the i threflected wave in region 1with wave vector k_{1i}. Likewise, the normalized total electricfield in region 3 is

$$E_3 = \sum_{i=-\infty}^{\infty} T_i \exp[-j\vec{k}_{3i}\cdot(\vec{r}-d\vec{z})] \quad (4)$$

where T_i is the normalized amplitude of the i th transmittedwave into region 3 with wave vector k_{3i} and d is the groovedepth. The quantities k_{1i} and k_{3i} are determined byusing the phase-matching requirement.

In RCWA, a series of layers parallel to the surface are introduced to explain the cross-section of the grating structure or the groove. Therelative permittivity for the n th slab grating is periodic, and may be expanded in a Fourier series as

$$\varepsilon_n(x,z_n) = \varepsilon_1 + (\varepsilon_3-\varepsilon_1)\sum_{h=-\infty}^{+\infty}\tilde{\varepsilon}_{h,n}\exp(jhKx) \quad (5)$$

where z_n is the z coordinate of the n th slab, h is the harmonicindex, K is the magnitude of the grating vector ($K = 2\pi/\Lambda$),and $\tilde{\varepsilon}_{h,n}$ are the normalized complex harmonic amplitudecoefficients given by

$$\tilde{\varepsilon}_{h,n} = (1/\Lambda)\int_0^{\Lambda} f(x,z_n)\exp(-jhKx)dx \quad (6)$$

where the function $f(x,z_n)$ is equal to either zero or unity,depending on whether, for a particular value of x, the gratingrelative permittivity is ε_1 or ε_3, respectively.

And the total field is thus expressed as

$$E_{2,n} = \sum_{i=-\infty}^{+\infty} S_{i,n}(z)\exp(-j\vec{\sigma}_{i,n}\cdot\vec{r}) \quad (7)$$

2.3 Finite element method (FEM)

FEM is a numerical technique tofind approximate solutions for boundary value problems in mathematics, which uses various methods (the Calculus of variations) to minimize an error function and produce a stable solution. Analogous to the idea that connecting many tiny straight lines can approximate a larger circle, FEM encompasses all the methods of connecting many simple element equations over many small subdomains, named finite elements, to approximate a more complex equation over a larger domain [13, 14, 15].

3. Method

In this paper, we use Rsoft and Comsol to obtain results from RCWA and FEM respectively. Use Matlab to solve effective RI of the mixture and Optilayer to calculate the reflectance of nanostructures using EMT.

4. Calculated results and discussion

The three theories provide us different methods to analyze and calculate the reflective characteristics of antireflective nanostructures. To make comparison of RCWA and EMT, the following results show that the two theories can prove each other.

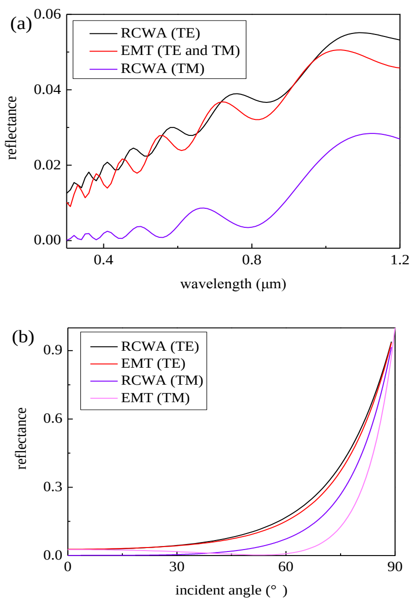

Fig. 3. Comparison of reflectance using RCWA and EMTin the model shown in Fig. 1 with $n_g = 3.48$, $\Lambda = 0.1\mu m$, $h = 0.5\mu m$, *(a) is with different wavelengths at normal incidence. Black curve is using RCWA for TE polarization and purple one for TM, red curve is using EMT for TE and TM polarization. (b) is with different incident angles at* $\lambda = 0.55\mu m$. *Black curve is for TE polarization and purple one for TM calculated by RCWA, red curve is for TE polarization and pink one for TM calculated by EMT.*

Fig. 3 shows comparision of reflectance using RCWA and EMT in the model shown in Fig. 1. Parameters are $n_g = 3.48$, $\Lambda = 0.1\mu m$, $h = 0.5\mu m$. Fig. 3 (a) is reflectance dependence on incident wavelength at normal incidence. Black curve is using RCWA for TE polarization and purple one for TM, red curve is using EMT for TE and TM polarization. As is shown, the R□λ curve calculated by EMT has the same behavior as that by RCWA in TE mode but differs 0.01~0.02 for reflectance in TM mode at normal incidence. Because for EMT, the antireflective nanostructureis supposed to be a number of lamellar grating layers with different filling factors and thereflectance can be analyzedusingthin-film theory, which is an approximate computation.Thus in the case of normal incidence, through EMT, the same results for both TE and TM polarizations were obtained from thin-film theory, but in actual nanostructures the results for TE and TM polarizations are different as calculated by RCWA. Fig. 3 (b) is the reflectance dependence on incident angle at $\lambda = 0.55\mu m$. Black curve is for TE polarization and purple one for TM calculated by RCWA. Red curve is using EMT for TE polarization and pink one for TM. As is shown, R□λ curve calculated by EMT is rather similar to that by RCWA at any incident angle in TE mode. However for TM mode, EMT is close to RCWA only if the incident angle is below 45°.

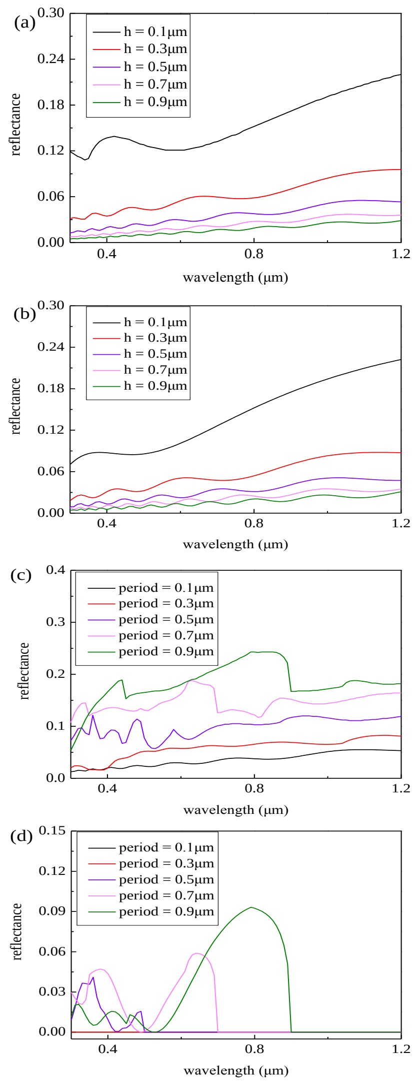

Fig. 4. Comparison of reflectance with different parameters at normal incidence of TE polarization, (a) is reflectance dependence on heights of the nanostructurewith n_g=3.48, Λ= 0.1μm *using RCWA, (b) on EMT, and (c)is total reflectance dependence on period of the nanostructure with c,* Λ= 0.1μm $h = 0.5um$ *using RCWA. (d) is reflectance of the + 1th order with* n_g=3.48, Λ= 0.9μm *and* h= 0.5μm *using RCWA.*

Fig. 4 shows reflectance dependence of wavelength for the nanostructures with different period and height calculated by EMT and RCWA, respectively. Fig. 4(a) shows the reflectance dependence on heights of the nanostructure calculated by RCWA, as is shown, the reflectance rises when the groove depth decreases, which is consistent with the results calculated by EMT shown in Fig. 4 (b), but they have rather small divergency, because for EMT more layers are introduced when the height gets larger, as a result, the gradient reflective approximation becomes more accurate. Fig. 4 (c)is total reflectance dependence on period of the nanostructure calculated by RCWA, as is shown, the reflectance rises when the period increases. Because higher order diffraction waves other than the zerothdiffraction order begin to propagate (as shown in Fig. (d)) when the period increases, which is a characteristics of gratings. These results above indicate that EMT is not suitable for large period ($>\lambda$) because higher order diffraction rather than zeroth order diffraction waves propagate now, which doesn't correspond to the thin-film theory. Fig. 4 (d) shows the reflectance of the +1th order, as a result, the +1th order wave begins to propagate when the period increases, but when the incident wavelength become rather larger, the +1th order disappears, therefore, only the zeroth order wave propagates.

RCWA provides an accurate analysis of diffraction of electromagnetic waves and computes rapidly, however unsuitable for non-periodical structures, that is to say we should suppose a calculation yieldrigorous periodical condition [4, 9].

To expound the progration of incident wave in nanostructure, FEM is adopted to give the distribution of E-field as is shown in Fig. 5.

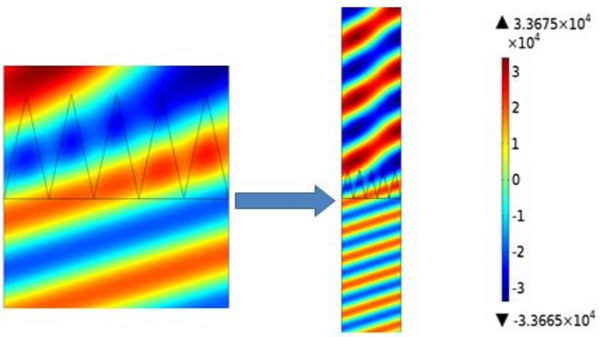

Fig. 5. Distribution of E-field (V/m) in the nanostructure at an incident angle of 30°.

In Fig. 5, the left schematic is an amplified schematic of E-field distribution in nanostructure based on the right one. We can see five units of period which is smaller than the incident wavelength. For a plane wave with TE polarization, it is obvious that through the nanostructure, light keeps its anterior character of propagation, so the reduction of reflectance in nanostructures is not due to the increase in diffuse scattering but solely the consequence of enhanced transmission. Hence, it is suitable to understand how EMT explains the phenomenon since EMT regardsnanostructureas a number of lamellar grating layers with gradient RIs which can be analyzedusingthin-film theory.

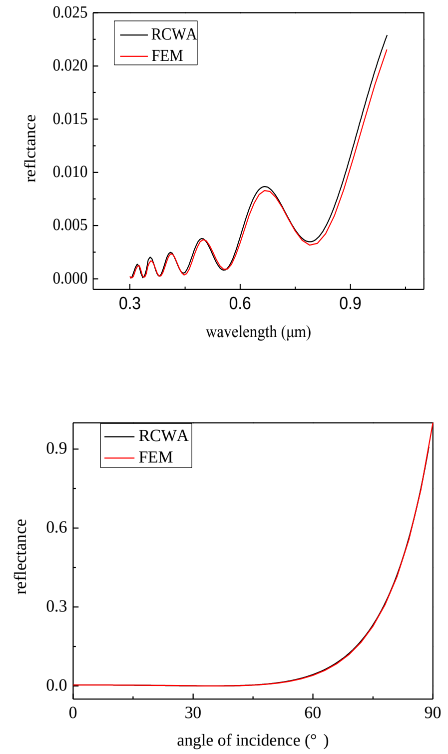

Fig. 6. Comparison of reflectance using RCWA (black curve) and FEM (red curve) with TM polarization and $h=0.5\mu m, \Lambda=0.1\mu m$. (a) is with different wavelengths at normal incidence, and (b) is with different incident angles at $\lambda=0.55\mu m$.

Fig. 6 shows the comparison of reflectance dependence on wavelength and angle of incident using RCWA (black curve) and FEM(red curve)with TM polarizationand $h=0.5\mu m, \Lambda=0.1\mu m$. As is shown, the computing results of the two theories are almost identical. To differentiate, FEM can deal with random structures however it has an excessive computation, and its working efficiency is in proportion to the dimension of calculation region.

5. Conclusion

This paper has analyzed different theories and made comparisons when dealing with the nanostructure. To choose a suitable method, conclusions are as follows.

When the period of nanostructure is larger than the incident wavelength, RCWA is the best choice because it works faster and accurately as well. FEM is accurate but with a massive computation. Besides, EMT is forbidden because only the zeroth order propagation is considered here while higher order propagations are not considered by EMT.

Else if the period is much smaller, RCWA and FEM are more accurate than EMT. For EMT, TE and TM polarizations have the same reflectance at normal incidence, however it's not the fact.

And in a non-periodic one, RCWA shouldn't be chosen as its calculating field must be periodic. EMT works best as FEM computes tediously.

Acknowledgements

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