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Antireflective Characteristics of Sub-Wavelength Periodic Structure with Square Hole *

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In order to enhance transmittance in the long-wavelength infrared range, the major parameters of periodic sub-wavelength structures (SWS) with square holes on zinc sulfide (ZnS) substrates are designed and analyzed for applications in normal incidence by using rigorous coupled-wave analysis (RCWA) and thin film theory (TFT). Finally the optimal antireflective parameters are achieved. The structures on ZnS substrates are fabricated on the basis of the simulation results by photolithography technology and reactive ion etching technology. A substantial antireflection effect is observed over the wavelength band 8–12 μm by a factor greater than 4.5.

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Zinc sulfide (ZnS) is one of the most promising long wavelength infrared (LWIR) materials with good mechanical and thermal properties as well as low IR absorption. However, the infrared reflection of the surface on ZnS is so high that it can not meet the demand of practical applications. Traditionally, thin films have been used to reduce unwanted reflection from the surface, but some problems such as thermal expansion mismatches and cohesion have been found to occur. An antireflective periodic sub-wavelength structure (SWS) is a promising method to suppress the reflection. This method can overcome the problems of thin films.

The period of antireflective SWS is smaller than the target wavelength and only the zero order diffraction occurs in SWS. In this manner the SWS acts as an effective medium covering the substrate.[1−3] Thus, SWS can mimic the effects of thin films.

SWS as an antireflection structured surface was discovered in nature on the cornea of night-flying moths by Bernhard in 1967.[4] This structure is potentially much cheaper and more durable than thin films. Moreover, SWS can be fabricated for special wavelength regions and incident angles. One-dimensional periodic SWS shows artificial birefringence and exhibits specific polarization in antireflection, where as two dimensional symmetrical periodic SWS is equivalent to uniaxial and less sensitive to polarization.[5] Previous experiments conducted to generate pillar arrays have successfully demonstrated infrared reflectivity reduction.[6−8] However, very few investigations have been carried out on antireflective SWS with hole.

In fact, both periodic SWSs of either square holes or square pillars can create an effective refractive index equal to the square root of the substrate materials' refractive index. The theory and experiment are the same except that the filling factors are reciprocal to each other, but the durability of periodic SWSs with square holes is better than periodic SWSs with square pillars.

In this Letter, we present theoretical work and experiment of SWSs with square hole on the ZnS substrate.

Three-dimensional view and unit platform view of SWSs with square hole are shown in Figs. 1(a) and 1(b), respectively. It is assumed that the thickness of the substrate is infinite, the period and the filling factor along the x and y axes are equal, i.e. $T_x = T_y = T$ and $a/T_x = b/T_y = f$.

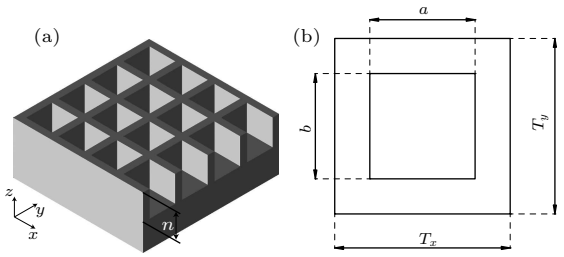

Fig. 1. Schematic diagrams of the square hole SWS surfaces: (a) three-dimensional view, (b) unit platform view.

In order to avoid the non-zero order diffraction from the periodic SWS for normal incident, the period should satisfy

$$T < \lambda_L / n_s, \tag{1}$$

where λ_L is the shortest wavelength of the target range and n_s is the refractive index of the substrate.

To facilitate fabrication, the critical dimensions of the antireflective SWS should be kept as large as pos-

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sible. According to inequality (1), the period for the ZnS substrate ($n_s = 2.2$) comes out to be $0.45\lambda_L$.

SWS can be modeled as a homogeneous thin film layer with index $n_{\rm eff}$.[5] According to the thin film theory (TFT), the refractive index $n_{\rm eff}$ and the depth h of SWS required for zero reflectivity should satisfy

$$n_{\rm eff} = \sqrt{n_s}, \tag{2}$$

$$h = \lambda/(4n_{\rm eff}), \tag{3}$$

where λ is the wavelength at which the transmittance maximum is to occur.

In order to enhance the broad-band transmittance, λ is defined as[9]

$$\lambda = 2\lambda_L\lambda_H/(\lambda_L + \lambda_H), \tag{4}$$

where λ_H is the highest wavelength of the target range.

For the ZnS substrate, the effective refractive index $n_{\rm eff}$ is 1.48 according to Eq. (2) and the initial depth is 0.17λ ($\lambda = 1.2\lambda_L$) according to Eq. (3). These parameters can be used initially for rigorous coupled-wave analysis (RCWA)[10–15] to achieve optimal parameters of SWS.

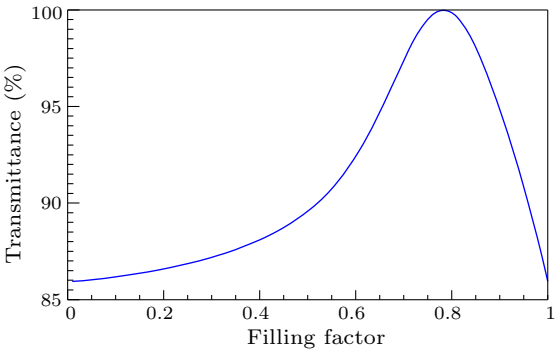

Fig. 2. Transmittance as a function of filling factor.

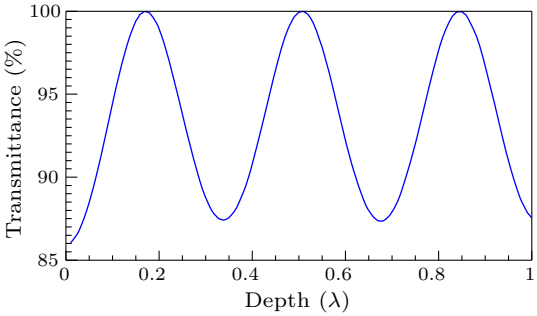

Fig. 3. Transmittance as a function of depth.

Figure 2 shows the transmittance as a function of fill factor for depth value of 0.17λ and period value of $0.45\lambda_L$ for normal incidence. As filling factor increases, the transmittance falls to a maximum value at $f = 0.78$. The effective refractive index of SWS corresponding to the value is 1.48. Further increasing the filling factor, the transmittance falls relatively sharp. Details of the curve shown in Fig. 2 are different for different profiles of SWS, because the equivalent index of SWS is determined by the volume fraction of the air in the corresponding layer.

Figure 3 shows the relationship between transmittance and depth for filling factor 0.78λ and period 0.45λ for normal incidence. Transmittance has a sinusoidal dependence on the depth and it cycles through minima and maxima as the depth increases. Transmittance has maximum value at depth value of 0.17λ, 0.51λ and 0.85λ. To facilitate fabrication, the depth should be kept as small as possible.

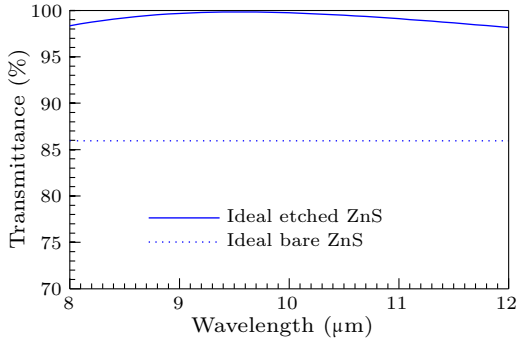

Fig. 4. Transmittance as a function of incident wavelength.

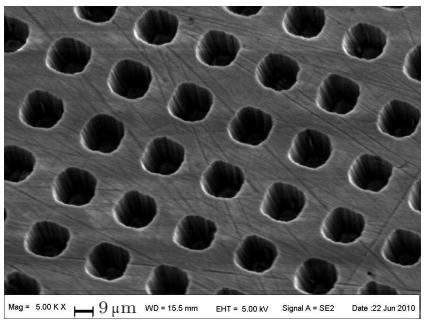

Fig. 5. SEM photomicrograph of etched SWS in the ZnS substrate.

For maximum transmittance over the waveband of 8–12 μm, the optimal period, depth and filling factor of SWS with square hole are 3.6 μm, 1.63 μm and 0.78, respectively, for the ZnS substrate.

Figure 4 shows the relationship between transmittance and incident wavelength for the optimal parameters. The increment of the average transmittance is 13.6% over the waveband 8–12 μm.

The optimal parameters are developed for etching SWS with square hole in $\phi 20\,{\rm mm} \times 5\,{\rm mm}$ thermopressed ZnS substrate. Figure 5 shows the single side etched SWS by the conventional photolithography technology and reactive ion etching technology with the gases $CH_4/H_2/Ar$.[16] The square hole array structures exhibits good anisotropic etching and only a slight tilt is seen in the sidewall. The etched depth is measured to be 1.60 μm and the etched filling factor

is measured to be 0.58.

Figure 6 shows infrared transmittance for spectra of the bare ZnS substrate and the single side etched ZnS substrate. Infrared average transmittance for bare ZnS substrate is 66.2% whereas infrared average transmittance for single side etched ZnS substrate is 70.7% over the waveband of 8–12 μm.

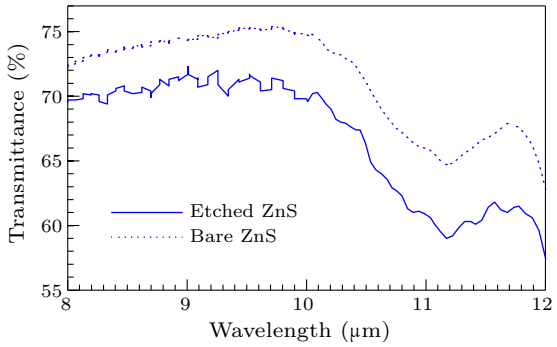

Fig. 6. Infrared transmittance spectra of the bare ZnS substrate and the single side etched ZnS substrate.

The increment of the average transmittance for spectra is 4.5% which is lower than the optimal value. The main problem is associated with the etched filing factor which is smaller than the designed value. The equivalent index of SWS is determined by the volume fraction of the air in that layer. The smaller the filling factor, the higher the equivalent index of SWS. Corresponding to the filing factor value of 0.58, the theoretical increment of transmittance is 4.65% for 9.6 μm, which is close to the experimental transmittance increment value of 4.2% for 9.6 μm. The reduced etch filling factor effects will reduce the transmittance and shift the peak of the transmittance to the right. In addition, the reflection on the background and the spectral absorption of the ZnS substrate also contributes to the reduced transmittance.

In conclusion, the broad band antireflective characteristics of square hole antireflective SWS are not so well as "moth eye" structure, but theoretically the special single wavelength transmittance of SWS can be increased to 100%, and also the depth of SWS is smaller than the depth of "moth eye" structure.[4] In this study, square hole antireflective SWS is investigated on a ZnS substrate; the optimal parameters are achieved for period 3.6 μm, depth 1.63 μm and filling factor 0.78 by RCWA and TFT. Then the structure exhibits good anisotropic etching and a close approximation to the optimal parameters (except for the filling factor) is fabricated by photolithography technology and reactive ion etching technology. The increment of the average transmittance for spectra is found to be 4.5% over the waveband of 8–12 μm.

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