Effects of Stress and Roughness on the Reflectivity of Blue Light in ZnS/MgF_2 Multilayers

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Abstract. The influences of stress and interface roughness on the reflectivity of blue light in the ZnS/MgF_2 multilayered film are evaluated quantitatively using the small deflection theory of elastic mechanics and the index method. The simulated results show that upon the interface roughness increasing, the reflectivity value of the blue light decreases but the shape of the reflectivity curve does not change. The applied stresses do not change the shape of the reflectivity curve. Depending on the compressive or tensile stress, the respective reflectivity curve shifts to right or left as compared to the one without stress, but such a shift depends strongly on the substrate thickness.

1. Introduction

The blue light that is part of the white light do have great harm to the human eye by damaging the light-sensing cells of retina [1]. Many efforts have been made to design a suitable optical multilayered film for filtering the blue light. To this end, the reflectivity of blue light in the prepared multilayered film is often evaluated quantitatively in order to obtain an optimum layered structure. On the other hand, to prepare a multilayered film on a foreign substrate, the interface roughness between sublayers and the stress between film and substrate may be introduced into the multilayered structure. Therefore, the effects of stress and interface roughness on the reflectivity of blue light in the multilayered structure have to be taken into account in order to obtain a reliable simulated result.

It was found that the interface roughness has a significant influence on the reflectivity by scattering losses, which has already been treated successfully both in theory and experiment [2]. Many papers in literature report the roughness effect on the optical properties for single layered structure [3] and for multilayered structure. Stress in thin film associated with the lattice mismatch and the difference of thermal expansion coefficient between film and substrate has also an impact on the reflectivity of optical thin film [4-5]. The stress may cause film crack and even falling off degrading the stability and the reliability of optical thin film. Currently, a couple of models have been put forward for analyzing the stress [6-11] such as the finite element method [12-14] and the boundary element method [15-16]. The stress in thin film is usually characterized by the curvature method [17].

In this paper, the influences of stress and interface roughness on the reflectivity of the blue light in

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the ZnS/MgF_2 multilayered film will be evaluated quantitatively using the index method and the small deflection theory of elastic mechanics. The zinc sulfide and magnesium fluoride are chosen because of the larger difference in their refractive index values.

2. Influence of interface roughness on the reflectivity

To simulate the reflectivity of an optical multilayered structure, a recursive method is often applied using an equivalent interface [18].

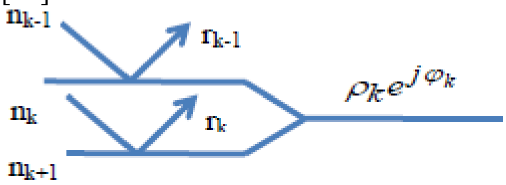

Figure 1. The equivalent interface of a single layer.

For a single layer, the equivalent interface is shown in Figure 1 and the corresponding reflection coefficient of this single layer is given by

$$r = \rho_k e^{i\varphi_k} = \frac{r_k + r_{k+1}e^{-j2\delta_k}}{1 + r_k r_{k+1}e^{-j2\delta_k}} \tag{1}$$

where r_k is reflection coefficient of the upper interface, r_{k+1} is reflection coefficient of the lower interface. The r_k can be obtained by the Fresnel expression for S polarization as

$$r_k = \frac{n_k \cos\theta_i - n_{k+1}\cos\theta_t}{n_k \cos\theta_i + n_{k+1}\cos\theta_t} \tag{2}$$

where θ_i is the incident angle, θ_t is the refracted angle. According to the Snell's law ($n_0 \sin\theta_0 = n_k \sin\theta_k = n_s \sin\theta_s$), the incident angle or the refracted angle can be calculated. n_k is the refractive index of the *k-th* layer.

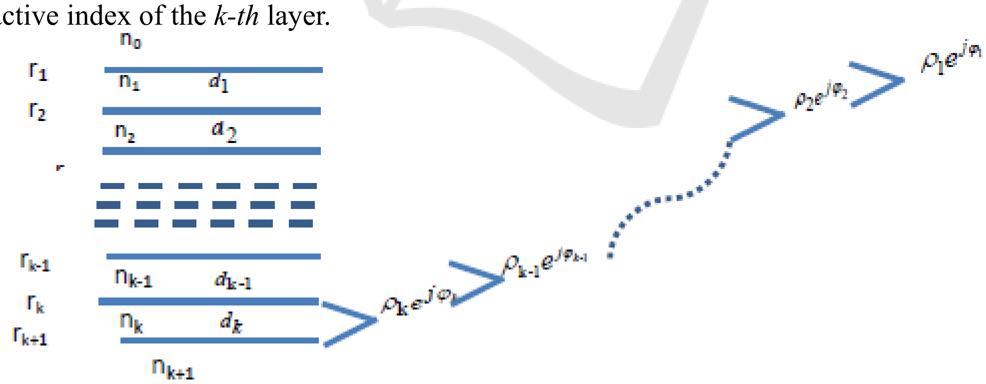

Figure 2. The recursive method for obtaining the Fresnel coefficient.

For a multilayered structure as sketched in the left side of figure 2, the equivalent interfaces are constructed as shown in the right side of Figure 2.

$$\rho_k e^{i\varphi_k} = \frac{r_k + r_{k+1}e^{-j2\delta_k}}{1 + r_k r_{k+1}e^{-j2\delta_k}} \quad \rho_{k-1} e^{i\varphi_{k-1}} = \frac{r_{k-1} + \rho_k e^{-j2\delta_{k-1}}}{1 + r_{k-1}\rho_k e^{-j2\delta_{k-1}}} \quad \ldots\ldots \quad \rho_1 e^{i\varphi_1} = \frac{r_1 + \rho_2 e^{-j2\delta_1}}{1 + r_1 \rho_2 e^{-j2\delta_1}} \tag{3}$$

where $\delta_j = \frac{2\pi}{\lambda} n_j d_j \cos\theta_j$ and d_j are the phase difference and the thickness of the *j-th* layer, respectively, λ represents the wavelength of incident light.

Then, the reflectivity of the multilayer can be calculated by

$$R = r \cdot r^* \tag{4}$$

To calculate the refraction index, the Sellmeier dispersion equation of equation (5) is used

$$n^2(\lambda) = A + \frac{B}{\lambda^2} \tag{5}$$

where, for the investigated material MgF_2, A=1.8976, B=0.01536 and for ZnS, A=5.013, B=0.2025.

When considering the effect of the interface roughness on the reflectivity of optical multilayers, two methods may be applied: the stratified-interface method [19] and the index method [20]. In the stratified-interface method, the rough interface is divided into different uniform thin layers, each layer has a homogeneous interface. As long as the divided layer is thin enough, the stratified-interface method can be used to describe well a rough continuous interface [19]. The index method is to calculate the Fresnel reflection coefficient at each interface where the interface roughness parameter is characterized by the real-structure model [21] and the Nevot-Croce model [20].

In the index method, the reflection coefficient at each interface of a multilayered structure is given by [20]

$$r_j = r_0 \exp\left[-\frac{1}{2}(q\sigma)^2\right] = r_0 M_j(q) \tag{6}$$

where $q = \frac{4\pi}{\lambda}\cos\theta_j$, $M_j(q)$ is called the Debye Waller factor, σ represents the interface roughness, θ_j is the incident angle, r_0 is the Fresnel reflection of the perfect interface ($\sigma = 0$). This method is applied to the case that the wavelength of the incident light is much large than the interface roughness [22-23]. For considering the influence of interface roughness on the reflectivity, the equation (2) will be replaced by the equation (6).

In the Real-Structure model [21], the interface roughness parameter is assumed to be increased with the depth from the substrate to the surface as demonstrated in Figure 3.

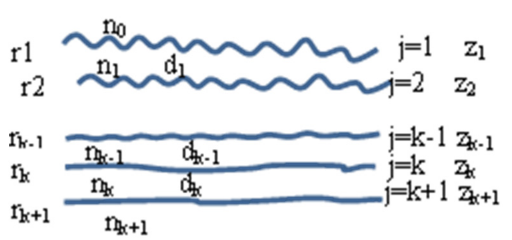

Figure 3. The sketch of the divided multilayer interfaces with different roughness characteristics.

The *j-th* interface roughness between the *j-th* and *(j +1)-th* sublayers is assumed as [22]

$$\sigma_j = \sqrt{\sigma_{k+1}^2 + h(z_{k+1} - z_j)} \tag{7}$$

where σ_{k+1} is the surface roughness of the substrate, z_{k+1} and z_j represent, respectively, the coordinate

values of the substrate's surface and the *j-th* sublayer's surface as shown in figure 3, h is a constant defined as the increase rate of interface roughness.
The factor $M_j(q)$ is given by

$$M_j = \exp\left[-\frac{1}{2}\left(\frac{4\pi\sigma_j}{\lambda}\right)^2 \cos\theta_j \cos\theta_{j+1}\right] \tag{8}$$

For $h = 0$ and $\sigma_{k+1} = 0$, it corresponds to an ideal interface.

3. Stress characterization

Due to the lattice mismatch between the film and the substrate, the film is constrained as shown in Figure 4.

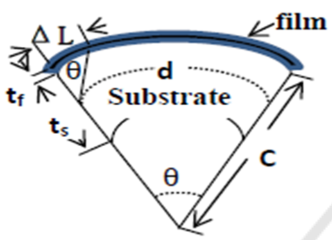

Figure 4. The sketch of the constrained film with the substrate. t_f is the film thickness, t_s is the thickness of the substrate. The middle plane of the substrate indicated as dashed line as no stress plane.

Assumed that t_s is much larger than t_f, and the stress in the film is regarded as a uniform distribution, the Stoney equation is expressed as [20]

$$\tau_f = \left(\frac{E_s}{1-\nu_s}\right)\frac{t_s^2}{6Ct_f} \tag{9}$$

where τ_f is the stress of surface, and C is the radius of curvature. In the z plane, the strain of xy plane is proportional to the distance z. Assuming that the Poisson's ratios of the film and the substrate are equal, namely, $\nu_s = \nu_s = 0.25$. While, for the glass substrate, the Es is equal to 55GPa. The packaging density P [24] is then described as

$$P = P_0(1 + 2kZ - 4\nu kZ)^{-1} \tag{10}$$

where k=1/C. Upon the curvature change, the refractive index can be rewritten as

$$n = n_0(1 + 2kZ - 4\nu kZ)^{-1} - (1 + 2kZ - 4\nu kZ)^{-1} + 1 \tag{11}$$

where n_0 is the refractive index of thin film material without stress. The equation (11) shows that the refractive index is associated with the distance Z from the middle plane of the substrate to the interface. Assuming that the substrate thickness is greater than that of the film and the refractive index of each sublayer is regarded as the same. Applying the equation (6) and (11) into the equation (2), the reflected coefficient of the multilayer can be calculated for considering the influences of both interface roughness and stress on the reflectivity.

4. Result and discussion

For the investigated refractive index materials, zinc sulfide and magnesium fluoride, using the

Genetic algorithm and truncation selection strategy, the optimum 4x ZnS/MgF_2 multilayered structure for the anti-reflectivity of the blue light is determined as 149, 29, 74, 31, 80, 33, 249 and 127 nm thick, respectively. In the following, the reflectivity of the above optimum multilayered structure will be calculated assuming that the incident light is perpendicular to the surface/interface, i.e. $\theta_0 = 0$.

4.1. Effect of roughness

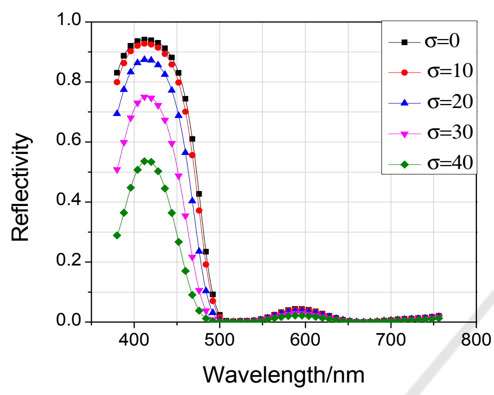

Figure 5. The reflectivity for different substrate roughness values with the same h value of 0.002.

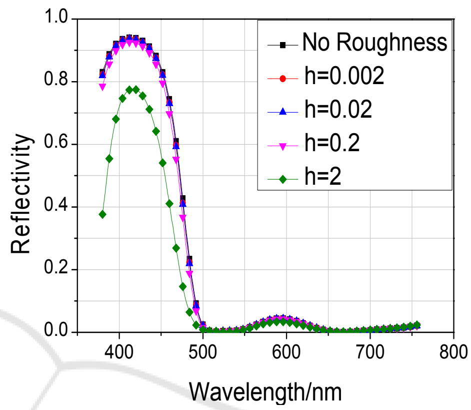

Figure 6. The reflectivity for the different h values with the same substrate roughness of 5nm.

Figure 5 shows that, with increasing the substrate roughness for the same *h* value of 0.002, the reflectivity of this multilayer is reduced. When the substrate roughness is less than 10 nm, the effect of roughness on the reflectivity can be ignored. However, when the substrate roughness is more than 40 nm, the maximum value of the reflectivity of the blue light is dropped significantly about 39% as compared to the ones for the roughness less than 10 nm. Upon the interface roughness increasing, the reflectivity value of the blue light decreases but the shape of the reflectivity curve does not change.

Figure 6 shows that, for the substrate roughness of 5 nm, the maximum reflectivity value decreases gradually with increasing of *h* value (the increase rate of interface roughness). But the interface roughness does not affect the reflectivity curve when the *h* value is less than 0.2. However, when the *h* value is of 2, the maximum reflectivity reduces about 15% but the shape of reflectivity curve does not change.

4.2. *Effect of stress*

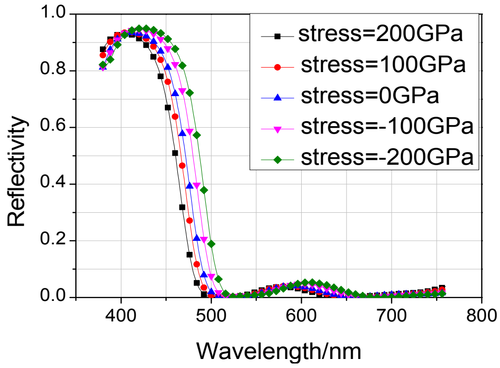

Figure 7. The reflectivity for different stress values with the same glass substrate thickness of 0.1 mm.

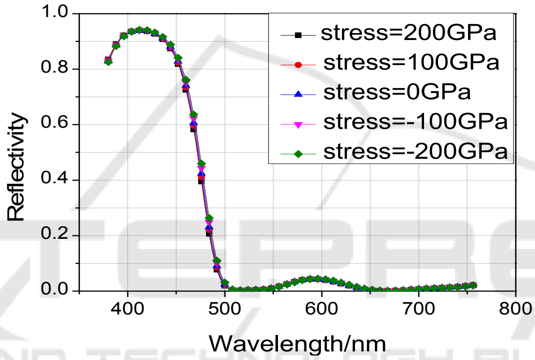

Figure 8. The reflectivity for different stress values with the substrate thickness of 1 mm.

In practice, stress value generally will not more than a few Gpa. The stress value here was set to 200 Gpa to show the impact of stress on the spectrum value. Figure 7 shows, when the glass substrate thickness is of 0.1 mm (the corresponding Young's modulus is 55 Gpa and the Poisson's ratio is 0.25), upon increasing the compressive or tensile stress value, the respective reflectivity curve shifts to the right or left as compared to the one without applied stress, but the shape the reflectivity curve remains the same.

However, when the substrate thickness increases to 1 mm, and all the other parameters including the applied stress values as indicated in Figure 7 remain the same, the reflectivity curve shown in Figure 8 does not change at all. It concludes that the influence of the applied stress on the reflectivity strongly depends on the substrate thickness. If the substrate thickness is thick enough, the applied stress in the multilayered film has no significant influence on the reflectivity of the blue light.

5. Conclusions

(1) Upon increasing the interface roughness, the reflectivity value of the blue light decreases, but the shape of reflectivity curve does not change;

(2) With increasing of the stress, the reflectivity curve shifts to the right or left as compared to the one without applied stress, but the shape of reflectivity does not change;

(3)The effect of stress on the reflectivity of the blue light could be ignored when the substrate thickness is thick enough.

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