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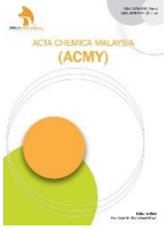

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RESEARCH ARTICLE

THEORETICAL STUDY OF OPTICAL PROPERTIES OF OPTICAL ANTI-REFLECTION FILMS

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ABSTRACT

In this paper, the theoretical calculation of the characteristics of the optical film, including the basic theory of the film, the calculation of the characteristics of the single-layer film, and the calculation of the characteristics of the multilayer film, to achieve a certain degree of understanding of the characteristics of the optical film. And through the optical anti-reflection film. The design principle, material selection, and process mastering have a deeper understanding of the anti-reflection film. The transmission spectrum is used to calculate the "envelope method" The refractive index, thickness, absorption coefficient, an extinction coefficient of the film to analyze the optical performance of the film.

KEYWORDS

Optical film, Optical anti-reflection film, Magnetron sputtering principle, TiO2 film

1. INTRODUCTION

As an important branch of modern optics, optical thin films have been widely used in industry, agriculture, construction, transportation, medicine, military, astronomy, infrared physics, laser technology, and other fields, playing an important role in people's daily work and life (Ai et al., 2021; Liu et al., 2019; Li et al., 2020). More and more important role. With the rapid development of science and technology, the rapid development of modern communication, energy utilization, aerospace technology and other fields, higher requirements are put forward for the development of optical thin film (Zhang et al., 2020; Li et al., 2020; Ma et al., 2018; Michael et al., 2016; Li and Yin, 2019; Ma and Tsai, 2017).

Since the 1970s, thin film technology has made rapid progress. Great achievements have been made in both academic and practical applications. Thin film technology has become the most active research field of vacuum technology and materials science. In the new technological revolution, the combination of thin film science, thin film materials and surface science promotes the comprehensive development and application of thin film products. From the perspective of development trends, the domestic and external thin-film industries are booming, and various signs indicate that thin-film technology will be there is a big breakthrough, which will drive the greater development of the film industry (Gao et al., 2018; Tsai and Ma, 2018; Li et al., 2020).

Over the past ten years, with the rapid development of thin film technology, the industry has made many greater breakthroughs, and with the development of various new materials, new functions have been discovered (Jiang et al., 2019). These have great development potential, and the latest technological revolution provides a reliable foundation (Liu et al., 2018; Li and Yin, 2019). Nowadays, besides a large number of electronic devices and large scale integrated circuits, thin film technology and thin film materials can also be used to support magnetic thin films and magnetic recording media, insulating thin films, dielectric thin films and piezoelectric thin films. The optical film, light guide mode, sensing film, wear-resistant, corrosion-resistant, self-lubricating film, decorative film, various special functions, etc. Anti-reflection film is the most important one of optical film, and its development has also been improved (Li et al., 2020). With people's extensive attention, the practical research of anti-reflection film has become a very meaningful work (Lin, 2013; Ma, 2017).

Anti-reflection film is used to reduce the reflection of the surface of the optical element and increase the light transmittance in the working band (Xie and Ma, 2018). The discovery of anti-reflection thin film in the 1930s promoted the early development of thin film optics (Zuo and Zhong, 2020). In order to promote the development of technical optics, anti-reflection films play the most important role among all optical films. Until today, in terms of the total amount of production, it still exceeds all other types of film (Guo et al., 2013).

The traditional optical glass industry, such as glass, lighting, automobile glass, modern optical fiber communication, photoelectric instruments, such as thermal imaging, low-light night vision, CCD camera photoelectric sensors, are constantly innovating, and the design and preparation requirements for improving the light transmittance in the working band are getting higher and higher. In the solar energy industry (Wu et al., 2021). In order to reduce the reflection loss of light on the cell surface and increase the light transmission, two main methods are used at present: (1) corroding the cell surface into a suede leather, and increasing the occurrence frequency of light on the cell surface. (2) one or more layers of anti-reflection coatings with matching optical properties are coated on the surface of the battery. The design of the anti-reflection coating directly affects the reflectivity of the solar cell to the incident light, and plays a very important role in improving the efficiency of the solar cell. Key Role (Li et al., 2020).

This demonstrates the importance of the anti-reflection film, so we must elaborate and analyze the problem.

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This article is mainly divided into three parts: the first part is about the theoretical calculation of the characteristics of the optical film; The second part is mainly about the selection of the material of the optical anti-reflection film and the design of the film system. The third part is mainly about the TiO2 film. The optical constant calculation and the single-layer SiO 2 anti-reflection coating layer have been initially realized.

2. BASIC THEORY OF OPTICAL FILM

The optical film consists of a thin layer of medium, which is a kind of visual medium material that propagates the light beam through the interface. The application of photosensitive thin film began in the 1930. Nowadays, optical thin film have been widely used in optical and photoelectric fields, and various optical Instruments are being manufactured.

Most optical films are designed according to optical interference theory, and various optical properties can be obtained by using optical interference. It can reduce surface reflection to increase the transmittance and contrast of the optical system, or increase the surface reflection to reduce the light and achieve the purpose of color separation and combination with high transmittance; It can also make light beams of different polarization states have different propagation characteristics and realize polarization beam splitting and polarization conversion. Below we will use the concept of the optical path difference to specifically Discuss the interference of the thin film.

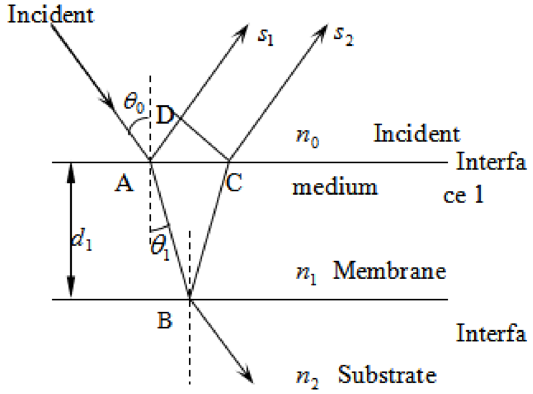


Figure 1: Thin film interference

As shown in Figure 1, 1 and 2 respectively represent the interface between the upper and lower surfaces of the film and other media, n_0 with n_2 Refractive index of the medium, n_1 Is the refractive index of the film, d_1 Is the thickness of the film. A monochromatic light at the angle of incidence θ_0 A part of the interface 1 incident on the film is reflected on the interface 1 with an amplitude of S_1 , The other part passes through interface 1, reflects on interface 2, and then passes through interface 1, the amplitude is S_2 .According to the laws of reflection and refraction, it is easy to prove that when the interfaces 1 and 2 are parallel, S_1 with S_2 The two reflected lights are parallel to each other. They will converge at infinity, causing interference. In the laboratory, you can use a convex lens to converge it on the focal plane to observe, of course, you can also directly observe it with your eyes.

Reflected light S_1 with S_2 The intensity of the interference depends on their optical path difference. According to the definition and geometric relationship of optical path difference, S_1 with S_2 The optical path difference is:

$$\Delta = 2n_1 \cdot AB - n_0 \cdot AD = \frac{2n_1 d_1}{\cos\theta_1} - 2n_0 d_1 \tan\theta_1 \cdot \sin\theta_0 \tag{1}$$

According to the law of refraction, there is

$$n_0 \cdot \sin\theta_0 = n_1 \cdot \sin\theta_1 \tag{2}$$

Substituting equation (2) into equation (1), we get

$$\Delta = 2n_1 d_1 \cos\theta_1 \tag{3}$$

The corresponding phase difference is

$$\delta = \frac{\Delta}{\lambda} \times 2\pi = \frac{4\pi n_1 d_1 \cos\theta_1}{\lambda} \tag{4}$$

If the phase jump when the light is reflected on the interface 1 and 2 is not considered first, then when the optical path difference meets the condition $\Delta = 2n_1 d_1 \cos\theta_1 = k\lambda, (k = 0,1,2,\cdots)$ At the time, constructive interference occurs, the amplitude is the largest after superposition, and the light intensity is the largest; when the optical path difference meets the conditions $\Delta = 2n_1 d_1 \cos\theta_1 = (2k-1)\frac{\lambda}{2}, (k = 0,1,2,\cdots)$ At this time, destructive interference occurs, the amplitude is the smallest after superposition, and the light intensity is the smallest.

In order to calculate the light intensity after interference superposition, set S_1 with S_2 The vibration equation of the two reflected lights is

$$\begin{aligned} E_1 &= s_1 \cos\omega t \\ E_2 &= s_2 \cos(\omega t - \delta) \end{aligned} \tag{5}$$

Therefore, the combined vibration after superposition is

$$E = E_1 + E_2 = s\cos(\omega t - \varphi) \tag{6}$$

among them, S Is the combined amplitude, φ Is the initial phase of the combined vibration. S_1 、 S_2 、 δ The relationship is as follows

$$s^2 = s_1^2 + s_2^2 + 2s_1 s_2 \cos\delta \tag{7}$$

$$\tan\varphi = \frac{s_2 \sin\delta}{s_1 + s_2 \cos\delta} \tag{8}$$

According to the definition of light intensity, the formula of double beam interference intensity is

$$I = I_1 + I_2 \pm 2\sqrt{I_1 I_2}\cos\delta \tag{9}$$

Among them, I, I_1, I_2 Are the combined vibration, S_1 with S_2 The intensity of $\pm$ Phase difference δ When the light is reflected from the light sparse medium to the interface of the light dense medium, there will be π Phase transition (often called half-wave loss). $\pm$ The number is precisely considering the phase jump when reflecting on the interface.

In fact, when the light beam is irradiated onto the flat film, the light beam will be reflected multiple times at the upper and lower interfaces of the film, thus generating a set of reflected light beams and a set of transmitted beams, as shown in picture 2.

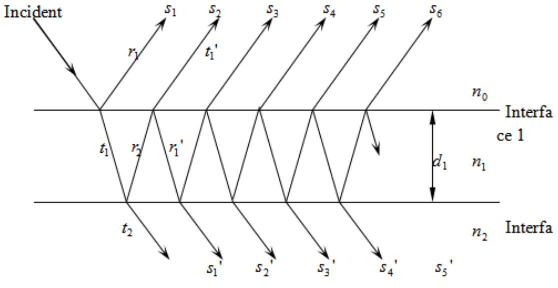


Figure 2: Multi-beam interference

When the reflection coefficient of the film surface is not high, usually only the first two reflected lights are considered S_1 with S_2 The effect of the reflected light beam that reflects the weak light intensity that reflects more than two times is ignored, that is, the multi-beam interference is treated as double-beam interference. However, if the reflectivity of the film surface is high, such treatment is not strict and must be considered. A set of reflected light $S_1, S_2, S_3, \cdots$ Or transmitted light $S_1', S_2', S_3', \cdots$ Multi-beam interference between.

The calculation method for the multi-beam interference light intensity is exactly the same as the double-beam interference. The vibration is first superimposed, and then the intensity is calculated. The difference is that the beam participating in the interference is increased from two beams to multiple beams. It is more convenient to use complex amplitude superposition. First calculate each reflected beam $S_1, S_2, S_3, \cdots$ Or transmitted beam $S_1', S_2', S_3', \cdots$ Amplitude and phase.

Let the amplitude reflection coefficients of the light reflected on the interface of 1 and 2 in the direction of the incident medium be respectively r_1, r_2, The amplitude transmission coefficient of the transmitted light is t_1'; The amplitude reflection coefficients of the reflected light in the direction of the substrate are: r_1', The transmission coefficients of the transmitted light are t_1, t_2 .when n_1 with n_2 When the medium is not absorbed, according to Stoke's law, there is

$$r_1 = -r_1' \tag{10}$$

$$r_1^2 + t_1 t_1' = 1 \tag{11}$$

According to the principle of superposition, the reflection coefficient of the combined amplitude of the reflected beams after superposition is

$$\begin{aligned} r &= r_1 + t_1 t_1' r_2 e^{-i\delta} + t_1 t_1' r_1' r_2^2 e^{-i2\delta} + t_1 t_1' r_1'^2 r_2^3 e^{-i3\delta} + \cdots \\ &= r_1 + \frac{t_1 t_1' r_2 e^{-i\delta}}{1 - r_1' r_2 e^{-i\delta}} \end{aligned} \tag{12}$$

Using equations (10) and (11), equation (12) can be written as

$$r = \frac{r_1 + r_2 e^{-i\delta}}{1 + r_1 r_2 e^{-i\delta}} \tag{13}$$

The intensity of the reflected light can be expressed by the reflectance, as

$$R = rr^* = \frac{r_1^2 + r_2^2 + 2r_1 r_2 \cos\delta}{1 + r_1^2 r_2^2 + 2r_1 r_2 \cos\delta} \tag{14}$$

According to the principle of conservation of energy, the transmittance is

$$T = 1 - R = \frac{(1 - r_1^2)(1 - r_2^2)}{1 + r_1^2 r_2^2 + 2r_1 r_2 \cos\delta} \tag{15}$$

As can be seen from the above formula, when $n_0 < n_1 > n_2$ Time, $r_1 < 0, r_2 > 0$, So the condition satisfied by the maximum transmitted light intensity should be $\delta = 2k\pi (k = 0,1,2,\cdots)$;when $n_0 < n_1 < n_2$ Time, $r_1 < 0, r_2 < 0$,and so $\delta = (2k+1)\pi (k = 0,1,2,\cdots)$ It is the condition that the transmitted light intensity is extremely small. The maximum and minimum conditions of the reflected light are exactly opposite to the transmitted light.

Generally, the anti-reflection film can be composed of a simple single-layer film or a multi-layer film system. The former can only make the light reflectivity of a certain wavelength band zero, while the latter can make the light reflectivity of a certain wavelength band zero. In general, it is required to enhance visible light, so it should adopt a multi-layer film structure. For the multi-layer film system, there is the recursive method, matrix method, and vector method. Although the combined admittance recursive method or matrix method is used to calculate the reflectivity of the film system is relatively strict and accurate, the calculation is too complicated, and it is not very effective to design the anti-reflection film. The simplest way to design the multi-layer film system is to use the vector method, first designing a more satisfactory structure through the trial method. Then use a computer to perform numerical calculations for accurate verification to eliminate the approximate effect inherent in the vector method. The vector method has two assumptions: one is the case that the film layer has no absorption; The other is that when determining the characteristics of the multilayer film, only consider a single reflection incident on each interface.

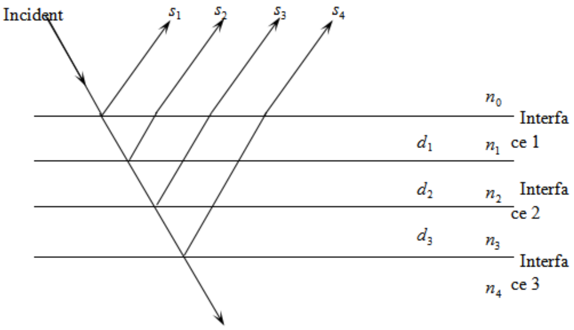


Figure 3: Reflection at the interface of the multilayer film

As shown in Figure 3, ignoring multiple reflections in the film, $S_1, S_2, S_3, \cdots$ Respectively represent the amplitude of the reflected light at each interface, and the reflection coefficient of each interface has a specific phase lag, which corresponds to the process of light entering the interface from the incident surface and returning to the incident surface. The amplitude reflection coefficient should be determined by the vector sum of the reflection coefficients of each interface. Therefore, the synthesized amplitude reflection coefficient is

$$r = r_1 + r_2 e^{-i\delta_1} + r_3 e^{-i(\delta_1 + \delta_2)} + r_4 e^{-i(\delta_1 + \delta_2 + \delta_3)} + \cdots \tag{16}$$

Among them $r_1, r_2 \cdots$ Respectively, the amplitude reflection coefficient of each interface, if the film layer does not absorb, the amplitude reflection coefficient of each interface is a real number

$$r_1 = \frac{n_0 - n_1}{n_0 + n_1}, r_2 = \frac{n_1 - n_2}{n_1 + n_2}, r_3 = \frac{n_2 - n_3}{n_2 + n_3}, r_4 = \frac{n_3 - n_4}{n_3 + n_4}, \cdots \tag{17}$$

The amplitude reflection coefficient can be positive or negative, depending on the relative size of the effective refractive index of the two adjacent media. If the dispersion of the film is ignored in the entire waveband considered, then for all wavelengths, the amplitude reflection coefficient $r_1, r_2 \cdots$ Are equal.

The phase lag of each film is

$$\delta_1 = \frac{4\pi n_1 d_1 \cos\theta_1}{\lambda}, \delta_2 = \frac{4\pi n_2 d_2 \cos\theta_2}{\lambda}, \delta_3 = \frac{4\pi n_3 d_3 \cos\theta_3}{\lambda}, \cdots \tag{18}$$

Therefore, the synthetic amplitude reflection coefficient can be obtained analytically, because the angle between two consecutive vectors is $\delta_1, \delta_2, \delta_3, \cdots$ Therefore, it is usually more convenient to use the vector illustration method to solve.

The steps of calculation using the vector method are: first calculate the amplitude reflection coefficient of each interface and the phase lag of each layer according to equations (17) and (18), draw each vector on the same polar coordinate diagram in proportion, and then press the triangle The law finds the sum vector. The modulus of the sum vector is the amplitude reflection coefficient of the film system, the amplitude angle is the phase change of the reflected light, and the energy reflectance is the square of the amplitude reflection coefficient.

3. DESIGN OF OPTICAL ANTI-REFLECTION FILM

The discovery of anti-reflection thin film in the 1930s promoted the early development of thin film optics. Promoting the development of technical optics, the anti-reflection film plays the most important role in all optical films. To this day, the total amount still exceeds all other types of film in number. Therefore, it is of great significance for production practice to study the design and preparation process of anti-reflection film.

Generally speaking, the selection of thin film materials should mainly observe the following characteristics: the transparent spectral region, transparency, refractive index, material evaporation method, mechanical robustness, chemical stability and high energy radiation resistance. Enter the properties of three thin-film materials commonly used: titanium dioxide, magnesium fluoride, and silica.

3.1 Titanium dioxide

Titanium dioxide (TiO_2) film has a high refractive index, a refractive index of 2.3 at a wavelength of 550 nm at 250°C, and a transparent area of 0.35 to 12 um It is transparent in the entire visible and near infrared spectral region. It has strong firmness and compressive stress. These excellent properties make it very attractive in optical films. However, TiO_2 material is in vacuum The phenomenon of oxygen loss due to heating is serious, and a high-absorption titanium oxide film Ti_nO_{2n-1} (n=1,2,...,10) is formed. So, in order to obtain high purity $Ti0_2$, we often use electron beam Direct evaporation of TiO_2, with the aid of ion source method, even at low temperature or even room temperature can get a relatively high refractive index, usually need to be filled with enough oxygen and maintain a high vacuum.

3.2 Silica

Silica (SiO2) is the only low-refractive-index oxide material with very small decomposition. When the wavelength is 550nm, the refractive index is 1.46, and the transparent region extends to vacuum ultraviolet (0.18~8um). Its light absorption is very small. The film layer is firm and resistant to abrasion and corrosion. It is extremely widely used. SiO2 is similar to TiO2 at high temperature evaporation, and can also produce low-priced oxides SiO and Si2O3. This low-priced oxide is often easier to evaporate than high-priced oxides, so the thin film It has a complex composition.The SiO2 film has a fine structure and is in a network-like glass state, which not only has small scattering and absorption, but also has strong protection ability.

When light enters another medium with a refractive index n1 from a medium with a refractive index n0, light reflection will occur at the interface between the two media. If the medium is not absorbed, the interface is an optical surface, and the light is vertical Incident, the reflectivity R is

$$R=(\frac{n_0-n_1}{n_0+n_1})^2 \tag{19}$$

If the absorption is not considered, the transmittance is t=1-r. For example, crown glass with a refractive index of 1.52 has a reflection of about 4.2% on each surface. Flint glass with a higher refractive index has a more significant surface reflection.

In order to reduce the reflected light on the surface, the simplest way is to coat a low refractive index film on the glass surface.

Let's take a look at a simple single-layer antireflection film. Let the thickness of the film bed. When the light is perpendicularly incident, the optical path difference of the reflected light on the two surfaces of the film is 2nd, because there is phase when reflecting on the upper and lower surfaces of the film. Sudden change, the result is no additional phase difference, when the two reflected lights interfere with each other, they should meet:

$$2nd=(2k+1)\lambda/2 \tag{20}$$

The minimum thickness of the membrane should be (corresponding to k=0):

$$d=\frac{\lambda}{4n}$$

Since the reflected light cancels, the transmitted light is strengthened.

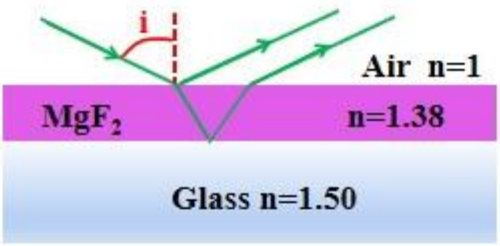


Figure 4: Glass-air critical diagram

The single-layer antireflection coating can only reduce the reflection of light of a certain wavelength λ as much as possible, and also reduce the reflected light of other wavelengths of similar wavelengths to varying degrees, but not to the weakest level. For general cameras and visual optical instruments, often Choose the most sensitive wavelength λ=550nm for human eyes as the "control wavelength". The lens looks at the reflected light of this film under white light, the yellow-green light is the weakest, and the red light and blue light are relatively strong, so the mirror surface is purple.

The reflectance at the center wavelength at this time $R=(\frac{n_0-n_1^2/n_2}{n_0+n_1^2/n_2})^2$

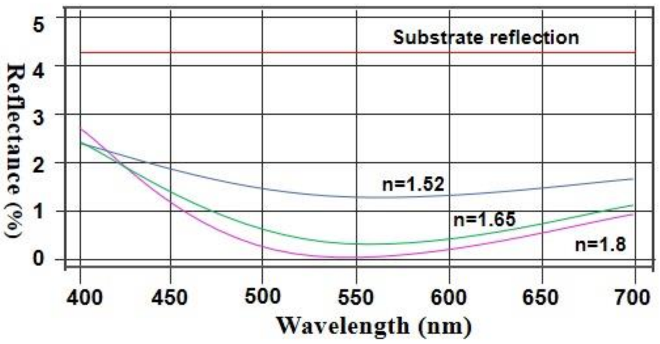


Figure 5: The residual reflection of MgF2 plated on different refractive index substrates

For glass with a refractive index of 1.52, after coating a single layer of MgF2 film with a thickness of 99.6 nm, the reflectance at the center wavelength of 550 nm can be reduced from 4.2% to about 1.3%, and the average reflectance of the entire visible light region is about 1.5%.

The emergence of a single-layer anti-reflection film is a major development in history. It is still widely used today to meet some simple uses. However, it has two major drawbacks. First, for most applications, the remaining reflection is still It seems too high; in addition, the light reflected from the uncoated surface remains neutral in color, while the light reflected from the coated surface disrupts the color balance.

There are basically two ways to improve the performance of a single-layer film, that is, either a so-called non-uniform film with a variable refractive index, or a multilayer anti-reflection film.

For a single layer of magnesium fluoride, the refractive index of the crown glass is too low. To this end, we can first coat a λ004 thick film with a refractive index of n2 on the glass substrate, then for the wavelength λ004 That is to say, the system in which the film and the substrate are combined can be equivalent by using an imaginary substrate with a refractive index of Y=n222ng. Obviously, when n2>ng, there is Y>ng. That is to say, first plate one on the glass substrate After a high refractive index λ004 thick film layer, the refractive index of the substrate seems to increase from ng to n222ng, and then coating a λ004 thick MgF2 film layer can play a better anti-reflection effect.

For example, for a substrate with a refractive index of 1.52, first deposit a layer of SiO coating with a refractive index of 1.70. At this time, Y=n222ng = 1.90, which is equivalent to the refractive index of the substrate increased from 1.52 to 1.90. Therefore, the MgF2 film just meets. The ideal anti-reflection conditions reduce the reflected light at a wavelength close to 0. However, for wavelengths that deviate from λ0 do not meet the condition of interference cancellation, the surface reflection will increase significantly, and the spectral reflectance curve is V-shaped, so this λ004-λ004 double-layer anti-reflection film is called V-shaped film.

In addition, the double-layer anti-reflection film with a thickness of λ004-

λ002 type is expected to have two minimum values of reflectance on both sides of the center wavelength λ0, and the spectral reflectance curve is w-shaped, so this double-layer anti-reflection. The film is called a w-shaped film. For the center wavelength λ0, the film layer with a thickness of λ002 is a dummy layer, which has no effect on the reflectance, but affects the reflectance of other wavelengths. Choosing the refractive index of the dummy layer appropriately can reduce. The refractive index on both sides of the center wavelength.

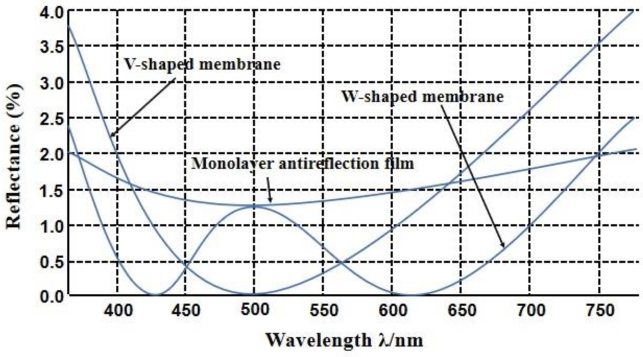
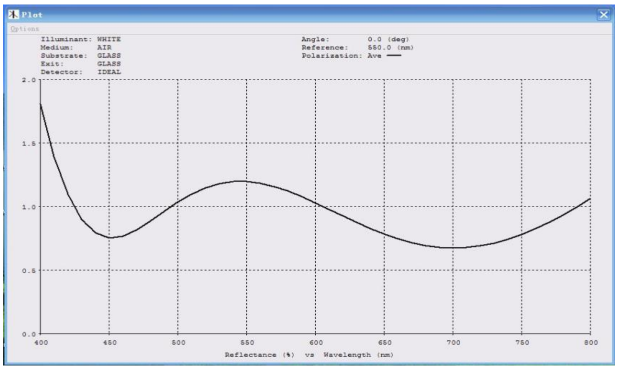


Figure 6: Reflections of different films

The performance of the double-layer anti-reflection film is much better than that of the single-layer anti-reflection film, but it does not overcome the above two defects of the single-layer anti-reflection film, especially for the crown glass.

As mentioned above, the characteristics of the double-layer anti-reflection film are much superior to the single-layer film. However, in many examples that can be used, even an ideal multi-layer film will still form excessive reflectance or Unsuitable spectral band width. Therefore, in these examples, three or more anti-reflection coatings are used.

For example, an Al2O3 film with a refractive index of 1.62 and a thickness of λ002 is first coated on a glass substrate, and then a MgF2 film with λ004 is coated. The reflectance curve is shown in Figure 7 below.

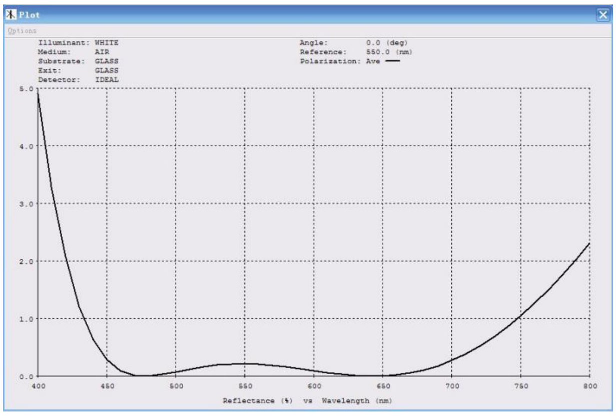


Illuminant: WHITE
Medium: AIR
Substrate: GLASS
Exit: GLASS
Detector: IDEAL

Angle: 0.0 (deg)
Reference: 550.0 (nm)
Polarization: Ave

Figure 7: MgF2 film reflectance curve

For example, a layer of CeF3 film with a thickness of λ004 is first coated on a glass substrate, and then a layer of ZnO film with a thickness of λ002, and finally a layer of MgF2 film with a thickness of λ004 is applied. The reflectance curve of the three-layer film is shown in Figure 8 below.



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Detector: IDEAL

Angle: 0.0 (deg)
Reference: 550.0 (nm)
Polarization: Ave

Figure 8: Three-layer film reflectance curve

4. CONCLUSIONS

In this paper, the theoretical calculation of the characteristics of the optical film, including the basic theory of the film, the calculation of the characteristics of the single-layer film, and the calculation of the characteristics of the multilayer film, achieve a certain degree of understanding of the characteristics of the optical film. And through the optical anti-reflection film the design principle, material selection, and process mastering have a deeper understanding of the anti - reflection film. The transmission spectrum is used to calculate the "envelope method" The refractive index, thickness, absorption coefficient, and extinction coefficient of the film, to analyze the optical properties of the film, through the study of the optical properties of the optical film, provides a theoretical guide for the preparation of optical devices.

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