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Research Article

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Determination of refractive index and thickness of YbF_3 thin films deposited at different bias voltages of APS ion source from spectrophotometric methods

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Abstract: Ytterbium fluoride (YbF_3) single thin films were prepared on sapphire and monocrystalline silicon substrates through conventional thermal evaporation and ion beam-assisted deposition (IAD), at bias voltages ranging from 50 to 160 V of the Leybold advanced plasma source (APS). By using the Cauchy dispersion model, the refractive index and thickness of the YbF_3 thin films were obtained by fitting the 400–2500 nm transmittance of the monolayer YbF_3 thin films on the sapphire substrate. At the same time, the refractive index and thickness of the YbF_3 thin films on the monocrystalline silicon substrates were also measured using the VASE ellipsometer at wavelength from 400 to 2200 nm. The results showed that the refractive index deviation of the YbF_3 thin films between the fitted values by the transmittance spectra and the measured values by the VASE ellipsometer was <0.02 and the relative deviation of the thickness was <1%. Furthermore, the refractive index of the YbF_3 thin films increased with increasing APS bias voltage. The conventional YbF_3 thin films and the IAD thin films deposited at low bias voltage revealed a negative inhomogeneity, and a higher bias voltage is beneficial for improving the homogeneity of YbF_3 thin films.

Keywords: bias voltage; refractive index; transmittance spectra; YbF_3 thin film.

OCIS codes: (310.0310) thin films; (310.6860) thin films; optical properties.

1 Introduction

Ytterbium fluoride, as a hard and environmentally stable material, has been extensively studied [1–6] and widely used as an optical coating in many practical applications because of its excellent transmittance from the ultraviolet (UV) to infrared (IR) ranges, low absorption, and low refractive index, such as in UV and IR lasers, high reflective mirrors, and anti-reflection coatings.

A good knowledge of the refractive index and absorption coefficient of the coating materials is essential to design and produce an optical multilayer interference filter [7, 8]. At present, some methods have been used to calculate the optical constants of thin films, such as spectrometry (extreme value method, envelope method, and full spectral fitting inversion method) [9–12], spectroscopic ellipsometry [13], polarization conversion [14], surface plasmon, and others [15]. Especially, the full spectral fitting inversion method is widely used because calculating the optical constants by the method does not require the relevant extreme point but only the transmittance of the film needs to be provided, and obtains the final result with relatively high precision.

In this paper, YbF_3 single thin films were deposited on sapphire and monocrystalline silicon substrates by using the conventional thermal evaporation method and advanced plasma source (APS)-assisted deposition. In addition, by using the Cauchy dispersion model, the refractive index and thickness of the YbF_3 thin films were obtained by fitting the 400–2500 nm transmittance of the monolayer YbF_3 thin films on the sapphire substrate. The results could provide a reference for the design and development of the corresponding optical thin film elements.

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2 Principles

2.1 Fitting refractive index of non-absorbing substrates

The double-sided transmittance of the non-absorbing substrate T in the case of normal incidence can be expressed as

$$T = 2n_s / (1 + n_s^2), \tag{1}$$

where n_s is the refractive index of the substrate and the refractive index of air is 1.

The Sellmeier equation is an empirical relationship between the refractive index and wavelength for a particular transparent medium, and can well describe the dispersion relation of the refractive index of sapphire [16, 17]. The refractive index of sapphire can be expressed by the Sellmeier dispersion formula of Eq. (2):

$$n(\lambda)^2 = A_0 + A_1\lambda^2 / (\lambda^2 - B_1) + A_2\lambda^2 / (\lambda^2 - B_2), \tag{2}$$

where A_0, A_1, A_2, B_1, and B_2 are coefficients to be fitted. The transmittance of the substrate can be measured, and the coefficients in Eq. (2) can be determined by fitting the transmittance of the substrate; therefore, the refractive index dispersion curve of the substrate can be obtained.

2.2 Fitting refractive index of homogeneous thin films

Figure 1 shows the schematic diagram of a single-layer uniform thin film system, where the refractive index of air, n_0, is 1; n_s is the refractive index of the substrate; d is the thickness of the thin film; and $N = n - ik$ is the refractive index of the thin film. In the case of normal incidence, the characteristic matrix of the thin film can be given by [18].

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} \cos\delta & i\sin\delta / (n - ik) \\ -i(n - ik)\sin\delta & \cos\delta \end{bmatrix} \begin{bmatrix} 1 \\ n_s - ik_s \end{bmatrix}, \tag{3}$$

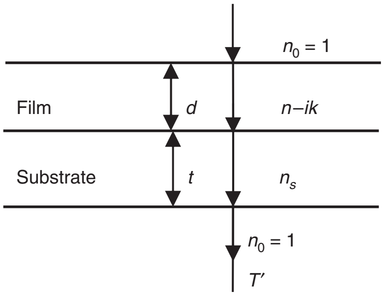

Figure 1: System of a thin film on a transparent substrate.

where $\delta = 2\pi(n - ik)d/\lambda$ is the phase thickness of the thin film. From Eq. (3), the optical admittance of the assembly (thin film and substrate) is $Y = C/B$ and the reflectivity of the thin film R is

$$R = \left(\frac{B - C}{B + C}\right)\left(\frac{B - C}{B + C}\right)^*. \tag{4}$$

The transmittance of the thin film T is

$$T = \frac{4n_s}{(B + C)(B + C)^*}. \tag{5}$$

T' denotes the double-sided transmittance (T' includes the reflection on the back of the substrate) and is expressed by

$$T' = \frac{TT_s}{1 - R_s R}, \tag{6}$$

where T_s and R_s are the transmittance and reflectivity of the interface between the substrate and air, respectively.

The double-sided transmittance T' contains all the information of the refractive index n of the thin film, the extinction coefficient k, and the thickness d. The double-sided transmittance T' of the thin film can be measured, and the appropriate dispersion model is selected. The thickness and dispersion parameters of the thin film can be obtained by fitting the measured transmittance. In the transparent band of the thin film, if the extinction coefficient is $k < 10^{-4}$, it usually can be negligible [18].

The transparent thin film in the visible and near-IR wavelength regions is the normal dispersion, and the Cauchy equation is usually used [19, 20]. The refractive index dispersion of the thin film can be expressed by the Cauchy dispersion formula of Eq. (7):

$$n(\lambda) = A_n + B_n / \lambda^2 + C_n / \lambda^4. \tag{7}$$

The coefficients A_n, B_n, and C_n in Eq. (7) can be determined by fitting the transmittance to obtain the refractive index dispersion curve of the thin film.

3 Experimental details

The YbF_3 thin films were deposited on sapphire and monocrystalline silicon substrates with a diameter of 30 mm and thickness of 3 mm. The samples were prepared with the ARES1510 high vacuum coating plant produced by Leybold Optics Company (Braunschweig, Germany), and were deposited by thermal evaporation with molybdenum boats. In the process of the deposition of the YbF_3 thin film samples, only the APS bias voltage changed from 50 to 160 V, the corresponding pressure in the chamber was below 8×10^{-6} mbar, and the deposited substrate temperature was 100°C. The deposition rate and the film thickness were monitored using a quartz crystal oscillator, and the deposition rate of YbF_3 was 0.5 nm/s. The substrate temperature of the YbF_3 thin film deposited by conventional thermal evaporation was 100°C.

The transmission spectra of the YbF_3 thin film samples on the sapphire substrate were measured using the Lambda900 spectrometer manufactured by Perkin Elmer (Hopkinton, MA, USA). The measured wavelength range was from 400 to 2500 nm, the wavelength interval was 1 nm, the accuracy of the transmittance measurement was 0.1%, and the shift downwards or upwards of the transmittance was ±0.1%. In order to verify the accuracy of the refractive index and thickness obtained by fitting, the refractive index and thickness of the YbF_3 thin film samples on the monocrystalline silicon substrates were measured using the VASE ellipsometer (J. A. Woollam, Lincoln, NE, USA). The measured wavelength was in the range of 400–2200 nm, and the accuracy of the refractive index was 0.005.

4 Results and discussion

4.1 Refractive index of substrate

In this paper, the refractive index of the substrate was calculated using the sample of φ30 mm × 3 mm sapphire, and the transmittance of the sample was measured using the Lambda900 spectrometer. The refractive index of the substrate was obtained by fitting the transmittance of the sample at the wavelength range of 400–2500 nm.

The Sellmeier dispersion coefficients of the sapphire substrate obtained by fitting were as follows: $A_0=2.51$, $A_1=5.78\times10^{-1}$, $B_1=3.36\times10^{-2}$ μm², $A_2=5.73\times10^{2}$, and $B_2=3.16\times10^{4}$ μm². The measured and the fitted transmittance of the sapphire substrate are shown in Figure 2. It can be seen from Figure 2 that the fitted and the measured transmittance are in good agreement. The refractive index of the sapphire substrate is shown in the solid line of Figure 3, and the broken line shown in Figure 3 is the refractive index in Ref. [21]. The deviation between the calculated refractive index of the sapphire substrate and that in Ref. [21] is small.

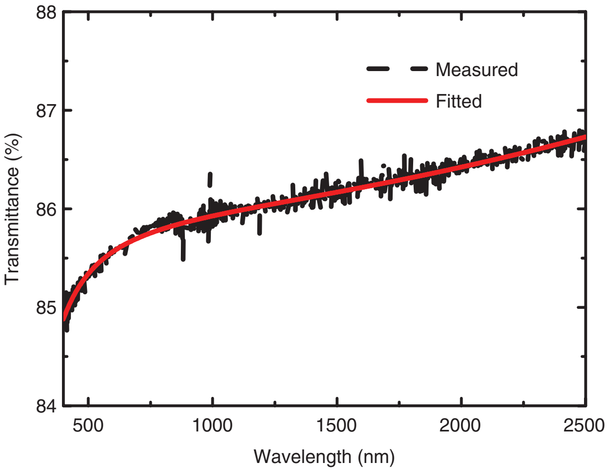

Figure 2: Transmittance of the sapphire substrate.

4.2 Refractive index and thickness of YbF_3 thin films

The Cauchy dispersion coefficient of the YbF_3 thin films obtained by the transmittance fitting are shown in Table 1, and the refractive index dispersion curve are shown in Figure 4. In Tables 1 and 2 and Figures 4 and 5, 0 V represents the YbF_3 thin films deposited by conventional thermal evaporation. Additionally, the refractive index of the YbF_3 thin films on the monocrystalline silicon substrates was measured using ellipsometry, as shown in Figure 4. The results show that the difference between the refractive index fitted by transmittance and that measured by ellipsometry is <0.02. It can be seen from Figure 4 that the refractive index of the YbF_3 thin films deposited by ion beam-assisted deposition (IAD) is higher than that of the YbF_3 thin films deposited by traditional thermal evaporation. The refractive index of YbF_3 thin films increased with increasing APS bias voltage. IAD can improve the packing density of the thin film, and the packing density of the

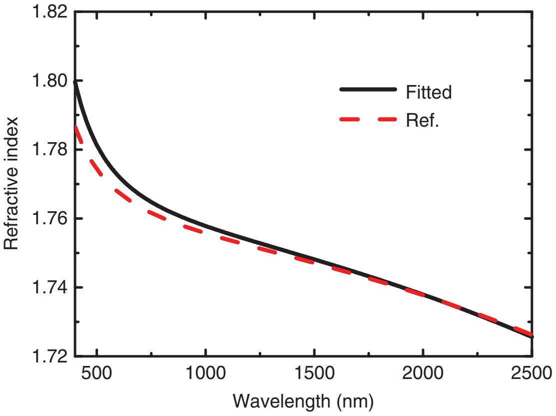

Figure 3: Refractive index of the sapphire substrate.

Table 1: Cauchy dispersion coefficient of the YbF_3 thin films.

	0 V (no APS)	60 V	120 V	160 V
A_n	1.4873	1.4904	1.5132	1.5156
B_n (μm²)	4.84×10^{-3}	4.89×10^{-3}	4.33×10^{-3}	4.37×10^{-3}
C_n (μm⁴)	5.68×10^{-5}	3.69×10^{-5}	4.15×10^{-5}	5.38×10^{-6}

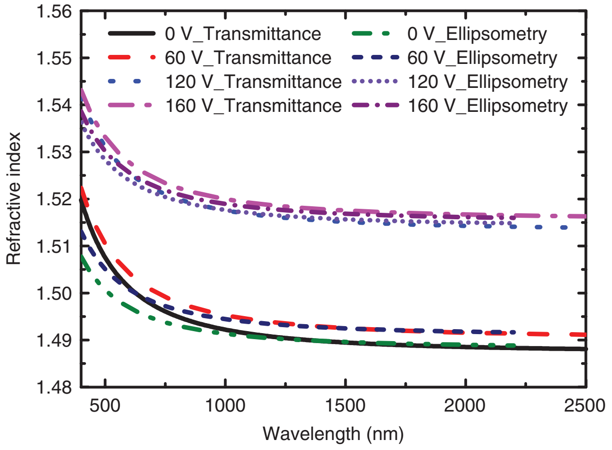

Figure 4: Refractive index of the YbF$_3$ thin films.

Table 2: Thickness of the thin films fitted by transmittance and thickness measured by ellipsometry.

	0 V	60 V	120 V	160 V
$t_{\text{transmittance}}$ (nm)	634.4	748.7	693.5	657.7
$t_{\text{ellipsometry}}$ (nm)	629.6	751.9	690.7	659.1
$t_{\text{transmittance}} - t_{\text{ellipsometry}}$ (nm)	4.8	−3.2	2.8	−1.4
$(t_{\text{transmittance}} - t_{\text{ellipsometry}})/t_{\text{ellipsometry}}$	0.76%	−0.43%	0.41%	−0.21%

thin film deposited by IAD was higher than that from the conventional thermal evaporation deposition. Correspondingly, the refractive index of thin film deposited by IAD was higher [5, 22].

The measured transmittance and the fitted transmittance of the YbF$_3$ thin films and the transmittance of the uncoated sapphire substrates are shown in Figure 5. Figure 5 shows that the fitted curve and the measured curve are in good agreement. For non-absorbent thin film, the change in the transmittance of the half-wave point being relative to the uncoated substrate is a reliable sign of inhomogeneity, and it can be used to measure inhomogeneity [23, 24]. The larger transmittance of the half-wave point deviating from the uncoated substrate means that the inhomogeneity of the thin film is greater. It can also be seen from Figure 5 that the deviation of the transmittance of the YbF$_3$ thin film from the traditional thermal evaporation method at the half-wave point near 2100 nm is the largest, and the bias voltage of 60 V follows. The bias voltages of 120 and 160 V have no significant deviation. Hence, a higher bias voltage is beneficial for improving the homogeneity of the YbF$_3$ thin films. The transmittance of the YbF$_3$ thin films by traditional thermal evaporation and bias voltage 60 V was higher than that of the substrate, which indicates that the YbF$_3$ thin films from the conventional thermal evaporation method and low bias voltage had negative inhomogeneity, i.e. the refractive index of the thin films decreased with increasing film thickness from the substrate to the surface of the layer. Figure 4 further shows that the deviation between the refractive index fitted by transmittance and that measured by ellipsometry of the YbF$_3$ thin films from traditional thermal evaporation at low bias voltage is larger than that at high bias voltage, which may be caused by the inhomogeneity of the thin films.

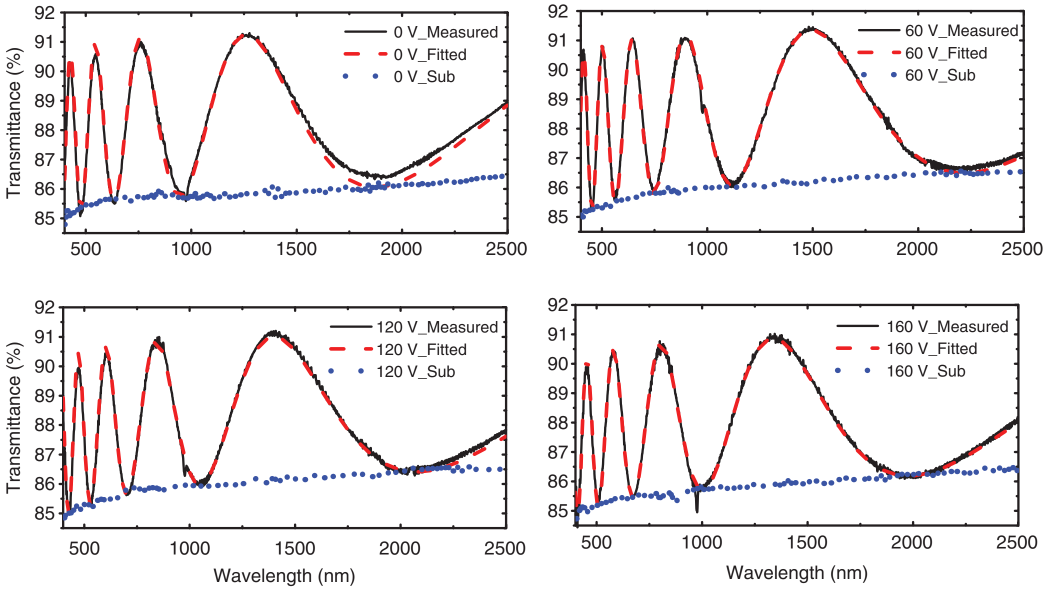

Figure 5: Transmittance of the YbF$_3$ thin films.

The thickness of the thin films fitted by transmittance and that measured by ellipsometry are shown in Table 2. The results show that the difference between the thickness by transmittance and that by ellipsometry is small and the relative deviation is <1%.

5 Conclusion

YbF_3 single thin films were deposited on sapphire and monocrystalline silicon substrates by using APS-assisted deposition and the traditional thermal evaporation method. Using the Cauchy dispersion model, the refractive index and thickness of the YbF_3 thin films in the wavelength range of 400–2500 nm were obtained by fitting the transmittance of the YbF_3 thin films on the sapphire substrate. At the same time, the refractive index and thickness of the YbF_3 thin films in the wavelength range of 400–2200 nm were measured using the VASE ellipsometer. The results showed that the deviation of the refractive index of the YbF_3 thin films between that fitted by transmittance and that measured by ellipsometry was <0.02 and the relative deviation of thickness was <1%. The refractive index of the YbF_3 thin film increased with increasing APS bias voltage. The conventional YbF_3 thin films and the IAD thin films deposited at low bias voltage revealed a negative inhomogeneity, and a higher bias voltage is beneficial for improving the homogeneity of YbF_3 thin films.

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