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Original research article

# Determination of infrared refractive index of ZnS and $YbF_3$ thin films by spectroscopy

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ABSTRACT

The refractive index of the infrared thin films was calculated by a relatively simple and accurate spectroscopy method. Using the Sellmeier dispersion model, the refractive index and thickness of the Zinc sulfide(ZnS) thin film were obtained by fitting the transmittance in the range of 2.5 μm–11 μm. At the same time, the refractive index and thickness of the ZnS thin films were also measured by VASE ellipsometer. The results show that the refractive index deviation between the values fitted by the transmittance and that measured by the VASE ellipsometer is $< 0.02$, and the relative deviation of the thickness is $< 1\%$.The $YbF_3$/ZnS bilayer coatings were deposited on the CVD Zinc selenide(ZnSe) substrate to obtain the refractive index of the ytterbium fluoride($YbF_3$) thin films wrapped in the coatings. Using the Sellmeier dispersion model, the refractive index of the $YbF_3$ thin film wrapped in the coatings was obtained by fitting the transmittance of the $YbF_3$/ZnS bilayer coatings in the range of 2.5 μm–11 μm. The results show that there are significant differences in the refractive index of the $YbF_3$ thin films wrapped in coatings and that exposed to the atmosphere.The refractive index of the $YbF_3$ thin film exposed to the atmosphere is abrupt because the $YbF_3$ thin films adsorbs water vapor, while that of the $YbF_3$ thin film wrapped in the coatings is no mutation.

## 1. Introduction

The thin-film materials are the basis for the preparation of optical films, and it is very important to accurately grasp the optical properties of thin film materials in the wide band range. The optical constants of the thin film are always affected by a number of factors such as deposition methods, process parameters and material properties [1–5]. At present, in order to obtain the optical constant of the thin film, firstly, the monolayer film is prepared under certain process conditions. Then, the optical constant of the films is solved by spectrometry (extreme value method, envelope method and full spectral fitting inversion method) [6–8], spectroscopic ellipsometry, prism-film coupler spectroscopy, surface Plasmon and polarization conversion, and others [9–13]. The full spectral fitting inversion method can obtain the optical constant of the thin film by fitting the transmittance or reflectance of the thin film. Furtherly, the inversion method requires only the transmittance or reflectance of the film, but not the relevant extreme point. Therefore, the inversion method is widely used [14,15].

In general, the $YbF_3$ thin film is a typical porous film, and the packing density is not very high. The $YbF_3$ thin film is exposed to air, and can adsorb water vapor, which may make its refractive index changed [16,17]. In the optical coatings, the $YbF_3$ thin film is often wrapped in coatings, not directly exposed to the air. The refractive index obtained by the monolayer $YbF_3$ thin film is different from

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that of the $YbF_3$ thin film wrapped in the coatings. Therefore, the refractive index of the $YbF_3$ thin film wrapped in the coatings has a practical significance for the design and preparation of optical coatings.

In this paper, using the Sellmeier dispersion model, the infrared refractive index of the ZnS thin film was obtained by fitting the 2.5 μm–11 μm transmittance of the monolayer ZnS thin film on the monocrystalline germanium substrate, and that of the $YbF_3$ thin film wrapped in the coatings was obtained by fitting the 2.5 μm–11 μm transmittance of the $YbF_3$/ZnS bilayer coatings on the CVD ZnSe substrate. The results can provide reference to design and develop the corresponding optical coatings elements.

## 2. Principles

### 2.1. Fitting refractive index of non-absorbing substrate

If the scattering of the substrate can be neglected, the double-sided transmittance of the non-absorbing substrate $T_0$ can be expressed as:

$$T_0 = (1-R_1)/(1+R_1) \tag{1}$$

where $R_1$ is the single-sided reflectivity of the substrate, and can be written as:

$$R_1 = (n_s-1)^2/(n_s+1)^2 \tag{2}$$

where $n_s$ is the refractive index of the substrate, and the refractive index of air is 1. The refractive index of the substrate in the infrared band can be expressed by the Sellmeier dispersion formula, i.e.:

$$n(\lambda)^2 = A_0 + A_1\lambda^2/(\lambda^2-B_1) + A_2\lambda^2/(\lambda^2-B_2) \tag{3}$$

where $A_0$, $A_1$, $A_2$, $B_1$, $B_2$ are coefficients to be fitted. The transmittance of the substrate in the infrared band can be measured, and the coefficients in the Eq.(3) can be determined by fitting the transmittance of the substrate. Then, the refractive index dispersion curve of the substrate can eventually be obtained.

### 2.2. Fitting refractive index of homogeneous thin films

Fig. 1 shows the schematic diagram of a multi-layer uniform thin film system. In the case of normal incidence, the characteristic matrix of the multi-layer thin film can be given by [18]

$$\begin{bmatrix} B \\ C \end{bmatrix} = \left\{ \prod_{i=1}^{K} \begin{bmatrix} \cos\delta_i & i\sin\delta_i/N_i \\ iN_i\sin\delta_i & \cos\delta_i \end{bmatrix} \right\} \begin{bmatrix} 1 \\ N_s \end{bmatrix} \tag{4}$$

where $\delta_i$ is the phase thickness of the $i$-th thin film; $N_i$ and $N_s$ are the complex refractive index of the $i$-th thin film and the substrate, respectively. The refractive index of air is assumed to be 1.

the reflectivity of the multi-layer thin film $R$ is

$$R = \left(\frac{B-C}{B+C}\right)\left(\frac{B-C}{B+C}\right)^* \tag{5}$$

the transmittance of the multi-layer thin film $T$ is

$$T = \frac{4N_s}{(B+C)(B+C)^*} \tag{6}$$

$T'$ denotes the double-sided transmittance ($T'$ includes the reflection on the back of the substrate), and can be expressed as

$$T' = \frac{TT_s}{1-R_sR} \tag{7}$$

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

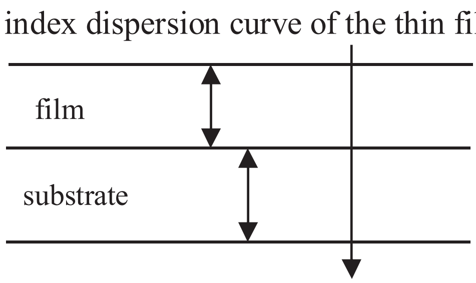


**Fig. 1.** System of a multi-layer thin film on a transparent substrate.