

Temperature coefficient of the refractive index for PbTe film

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Received September 20, 2016; accepted January 13, 2017; posted online February 14, 2017

Specimens of PbTe single film are deposited on Ge substrates by vacuum thermal evaporation. During the temperature range of 80–300 K, the transmittance of a PbTe film within 2–15 μm is measured every 20 K by the PerkinElmer Fourier transform infrared spectroscopy cryogenic testing system. Then, the relationship between the refractive index and wavelength within 7–12 μm at different temperatures is received by the full spectrum inversion method fitting. It can be seen that the relationship conforms to the Cauchy formula, which can be fitted. Then, the relationship between the refractive index of the PbTe film and the temperature/wavelength can be expressed as $n(\lambda, T) = 5.82840 - 0.00304T + 4.61458 \times 10^{-6}T^2 + 8.00280/\lambda^2 + 0.21544/\lambda^4$, which is obtained by the fitting method based on the Cauchy formula. Finally, the designed value obtained by the formula and the measured spectrum are compared to verify the accuracy of the formula.

OCIS codes: 310.6860, 120.4530, 160.4670.

doi: 10.3788/COL201715.043101.

As an important part of the optical system, infrared optical film directly determines the image quality of the system^[1–4]. Under cryogenic conditions in a space environment, its spectrum will drift significantly compared with the normal temperature, which is mainly caused by the temperature coefficient of the refractive index for an optical thin film^[5–7]. This change will have a significant impact on the optical system, and even make it a failure for a lofty precision optical machine, which required little change of performance with the temperature. PbTe film is widely used in infrared optical film, especially in the far infrared region due to its interesting properties, such as a high refractive index and wide transparent region^[8–11]. Currently, the refractive index of PbTe film under cryogenic conditions is commonly obtained by the fitting method and extrapolation^[12–14]. However, it is relatively poor in the terms of accuracy and efficiency, which would make sense in addressing these problems in the context of advanced manufacturing of the high precision infrared optical film.

This work is aimed at establishing a formula that can obtain the refractive index of PbTe film rapidly under different temperatures in a transparent region. By measuring the spectral transmittance of PbTe film, it is derived from the refractive index and the parameters of the Cauchy dispersion formula at different temperatures from 80 to 300 K. Then, the relationship between the parameters and the temperatures were obtained by numerical fitting. Finally, the relationship between the refractive index of PbTe film and the temperature/wavelength was received, and the accuracy of the formula was verified.

The interference effect can be produced when the lights spread in the transparent film. The spectral transmittance

through the monolayer film can be expressed as $t = 4n_0n_s/|n_0B + C|^2$ ^[12,15], where $\begin{pmatrix} B \\ C \end{pmatrix} = \begin{pmatrix} \cos \cos \alpha & \frac{i \sin \sin \alpha}{N} \\ iN \sin \sin \alpha & \cos \cos \alpha \end{pmatrix} \begin{pmatrix} 1 \\ n_s \end{pmatrix}$, $\alpha = 2\pi Nd/\lambda$, $N = n - ik$, λ is the incident wavelength, and n_0 and n_s are the refractive indices of the air and substrate, respectively. It is obvious that transmittance t is a multivariate function of the parameters n , k , and d of the thin film. Based on the extremum T_{\max} and T_{\min} of the spectrum, according to the theory of optical film, the refractive index of the film can be expressed as

$$n_f = [A + (A^2 - n_0^2 n_s^2)^{1/2}]^{1/2}, \quad (1)$$

where $A = n_0^2 + n_s^2/2 + 2n_0n_s(1/t_{\min} - 1/t_{\max})$, and n_0 and n_s are the refractive indices of the air and substrate, respectively.

As the initial value, the result of Eq. (1) is used to calculate the value of the refractive index of the film; meanwhile, the designed thickness was taken as the initial thickness of the film. Then, the wavelength range $\lambda_{\min} \sim \lambda_{\max}$ is divided into S intervals. The evaluation function is constructed by the difference between the actual measured value $\tilde{t}(\lambda)$ and the theoretical value of $t(\lambda)$, using the minimum of Merit as the objective function to get the optical parameters of the interval I , where the range of the optical parameters of the film is set as the constraint condition to construct the physical model of the optimization problem

$$\min \text{Merit}(i) = \int_{\lambda_{lb_i}}^{\lambda_{ub_i}} \omega(\lambda) [t(\lambda) - \tilde{t}(\lambda)] d\lambda, \quad (2)$$

$$\text{s.t.} \begin{cases} n_{lb_i} \leq n_i \leq n_{ub_i} \\ d_{lb_i} \leq d_i \leq d_{ub_i} \end{cases}, \quad (3)$$

where Eq. (2) is the objective function, Eq. (3) is the constraint condition, the lower and upper bounds of interval i are λ_{lbi} and λ_{ubi} , respectively, and $\omega(\lambda)$ is the weight factor of λ . An integrated optimization algorithm based on the nonlinear least squares method and the improved genetic algorithm is used to solve the physical model. Then, the optical parameters of interval i were obtained. Finally, the optical parameters of the remaining S-1 intervals can be received in turn, and more importantly, we get the optical parameters of the whole wavelength range of the film.

Specimens of the double-sided polishing (100)-oriented single crystal germanium wafers with the resistivity of $\sim 35 \Omega \cdot \text{cm}$ and a size of $15 \text{ mm} \times 15 \text{ mm}$ were selected as substrates. Then, the PbTe single film with its design thickness of 750 nm was coated on Ge substrates by the method of vacuum thermal evaporation using a Denton automatic optical coating machine. During the coating process, the vacuum was $3.0 \times 10^{-3} \text{ Pa}$, the deposition temperature was 523 K, the deposition rate was 1 nm/s, and the evaporation current was 120 A. Lastly, the transmittance of the PbTe single film within 2–15 μm was measured every 20 K by the PerkinElmer Fourier transform infrared spectroscopy (FTIR) cryogenic testing system within a temperature range of 80–300 K.

The transmitted spectra of the PbTe film at 80, 140, 200, 260, and 300 K are shown in Fig. 1. As we can see, the peaks and valleys of the spectrum are entirely drifting towards a long wavelength with the temperature decreasing. The drifting distance of the peak with a longer wavelength is much smaller than the valley. This can be ascribed to the negative temperature coefficient of the refractive index for PbTe film, which leads to a spectra red shift at a low temperature. Meanwhile, the change rate of the refractive index of PbTe with the temperature is quicker in a short wavelength region than in a long wavelength region. In addition, the short wavelength absorption edge red shifted to 5 μm from 3.5 μm when the temperature decreased to 80 K from 300 K due to the narrower energy band gap.

Figure 2 shows the relationship between the refractive index and the wavelength obtained by the full spectrum

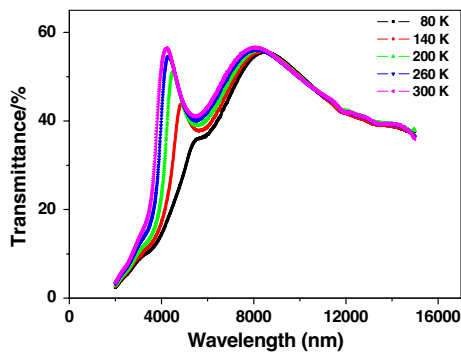


Fig. 1. The transmitted spectra of PbTe film at 80, 140, 200, 260, and 300 K.

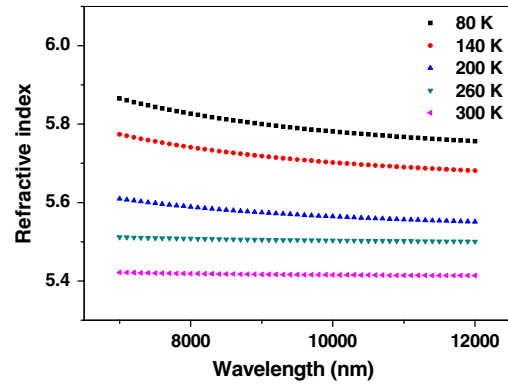


Fig. 2. The relationship between the refractive index and wavelength at 80–300 K, during the range of 7–12 μm .

inversion fitting method at 80–300 K during the range of 7–12 μm . It can be seen that the refractive index of PbTe film decreases with an increasing wavelength, and the change trend is almost the same at different temperatures. Moreover, it is received that the relationship between the refractive index and wavelength conforms to the Cauchy formula, which can be used by the fitting method.

The Cauchy formula can be expressed as $n(\lambda) = A_n + \frac{B_n}{\lambda^2} + \frac{C_n}{\lambda^4}$, where there are three unknown parameters A_n , B_n , and C_n ^[12]. Then, the relationships between the unknown parameters and the temperature T are researched below.

The relationship between A_n and T obtained by the binomial fitting method is shown in Fig. 3. It can be expressed as $A_n = 5.82840 - 0.00304T + 4.61458 \times 10^{-6} T^2$, where the square of correlation coefficient R is 0.99241, and the standard error is 0.00897. So, the difference between $A_{n \text{ max}}$ and $A_{n \text{ min}}$ is 0.2616 during temperature range of 80–300 K, and the temperature coefficient of A_n is -0.00108 K^{-1} .

The relationship between B_n/C_n and T are shown in Fig. 4. It can be seen that the temperature has little effect on B_n and C_n , which can be taken as an average of their value, respectively. The maximum effects of the B_n and C_n on the temperature coefficients of the refractive index for PbTe film are -1.98×10^{-6} and $-3.05 \times 10^{-8} \text{ K}^{-1}$.

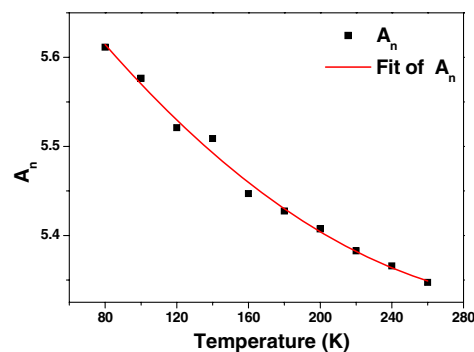


Fig. 3. The relationship between A_n and T .

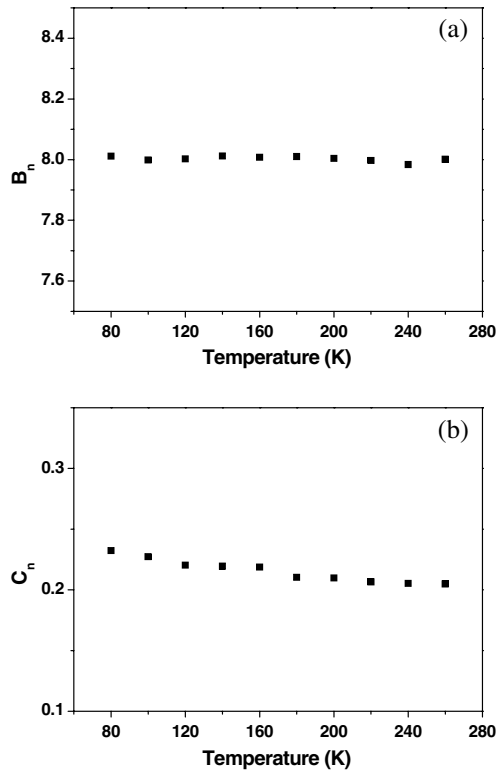


Fig. 4. The relationships between (a) B_n and (b) C_n and T .

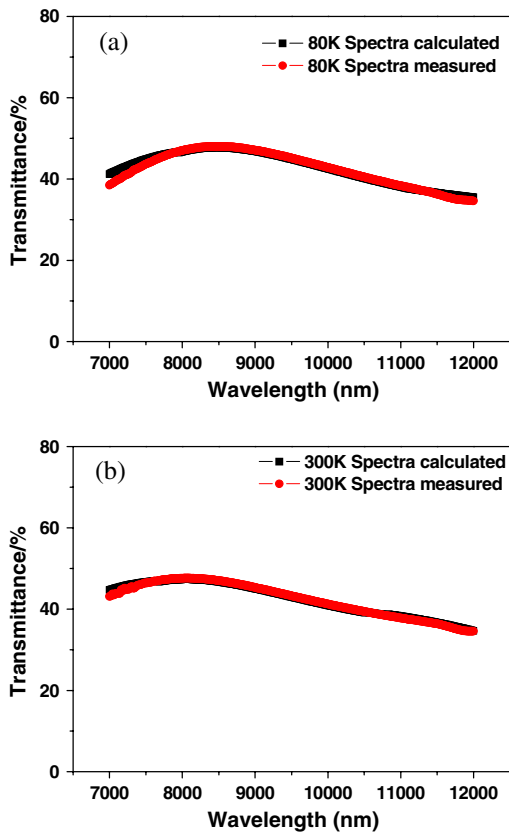


Fig. 5. The contrast of the designed spectra by the formula and the measured spectra at (a) 80 and (b) 300 K.

Based on the above analysis, the relationship between the PbTe film's refractive index and temperature/wavelength was obtained by the fitting method based on the Cauchy formula that can be expressed as

$$n(\lambda, T) = 5.82840 - 0.00304T + 4.61458 \times 10^{-6}T^2 + 8.00280/\lambda^2 + 0.21544/\lambda^4. \quad (4)$$

Moreover, the temperature coefficient of the refractive index for PbTe film is approximately equal to -0.00108 K^{-1} .

Figure 5 shows the contrast of the designed spectra by the formula and the measured spectra at 80 and 300 K. As we can see, the measured spectra coincide exactly with the designed value at 80 and 300 K within the region of 7–12 μm , which illustrate the accuracy of the temperature coefficient of the refractive index for PbTe film.

In conclusion, we obtain the relationship between the refractive index of PbTe film and the temperature/wavelength. The formula is established by the fitting method based on the Cauchy formula. The temperature coefficient of the refractive index for PbTe film is approximately equal to -0.00108 K^{-1} . These results can be used to calculate the refractive index of PbTe film at different temperatures within the range of 7–12 μm , which is beneficial for the fabrication of optical devices with high temperature stability.

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