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Study on characterization method of optical constants of germanium thin films from absorption to transparent region

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ABSTRACT

In this paper, the physical dispersion model of the optical constants of the amorphous germanium thin films was studied. Based on the Cody-Lorentz model, the optical constants of the films are characterized from the visible region to the long-wave infrared region. The optical constants are calculated from the inverse calculation of the reflection spectrum and the transmission spectrum in visible region. The calculated optical constants are extended to the infrared transparent region of the germanium thin films, which is consistent with the actual measurement results. The calculated optical constants are verified by the Cauchy model in the transparent region. According to the properties of band gap and tail width, the physical mechanism why the refractive index and extinction coefficient of films is greater than that of bulk material was determined. The decay rate of the germanium film in the long wave direction is lower than that of the germanium crystal due to the presence of the tail state in the germanium film material. Therefore, the refractive index and extinction coefficient of the film are greater than those of the bulk material.

1. Introduction

The germanium thin films is a typical indirect-band-gap semiconductor material, whose characteristics are usually between metal and insulator. It has high mechanical strength, good chemical stability and a long transparent region from 2 μm to 14 μm. Due to those advantages mentioned above, germanium are commonly used on lenses and window elements in the field of infrared imaging detecting technology. For instance, it is usually used as a high refractive index film of multilayer film element, such as antireflection films, high reflective films, the spectroscopic films and the filtering films [1–4].

The optical constant of the film is the key parameter to realize the function of the optical film. The Cauchy model and the Sellmeier model are the common physical dispersion models for obtaining the optical constants in the transparent region of the germanium film [5]. The optical constants are calculated from the inversion of the reflectance spectral or transmittance spectral. However, this method cannot obtain the structure characteristic and optical constants in the shortwave region. Forouhi and Bloomer reported the dispersion relationship of the amorphous and semiconductor thin films [6,7]. The F-B model is extended to the polycrystal thin films which have a clear physical meaning. In order to overcome the drawbacks of the F-B model, Jellison and Modine proposed the Tauc-Lorentz dispersion model for amorphous semiconductors and insulator materials [8,9]. And then Fersauto et al. proposed the Cody-Lorentz model based on the Tauc-Lorentz dispersion model [10,11] which incorporates the properties of band tail state of the amorphous material and gives the expression of the dielectric constant with the photon energy less than the band gap. Germanium thin film is a typical semiconductor thin film, a large number of paper reported the preparation methods and characteristics of germanium thin films. However, the optical constants of the germanium thin films in the shortwave regions are rarely reported.

Based on the Cody-Lorentz model, the optical constants of the germanium thin films prepared by electron beam evaporation were calculated from the reflection spectrum and the transmission spectrum (from visible to near infrared band). Compared with the Cauchy model, not only the optical constants and bandgap properties of the transparent region were obtained, but also the physical mechanism that why the refractive index of the film is higher than that of the bulk material can be explained.

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2. Physical model of optical constants

The germanium thin films are generally prepared by the thermal evaporation technology. For amorphous semiconductor materials, Ferlauto et al. [10] studied the band tail absorption and added it to the dispersion model. They proposed the Cody-Lorentz model and applied it to typical amorphous semiconductor materials. The imaginary part of the dielectric function is as follows:

$$\varepsilon_2(E) = G(E)\frac{AE_0\Gamma E}{(E^2 - E_0^2)^2 + \Gamma^2E^2}, \quad E > E_t$$
$$= \frac{E_1}{E}\exp\left[\frac{(E - E_t)}{E_u}\right], \quad E \le E_t \tag{1}$$

$$G(E) = \frac{(E - E_g)^2}{(E - E_g)^2 + E_p^2} \tag{2}$$

$$E_1 = E_t G(E_t) L(E_t) \tag{3}$$

where E_O, A, E_g and Γ are resonance energy, the Lorentz oscillator amplitude, band gap energy and oscillator width, respectively. While E represents photon energy (ev). E_t is the demarcation between the Urbach tail transitions and the band-to-band transitions. The tail transition occurs in the region where the photo energy is less than E_t, while the interband transition occurs in the region where the energy is greater than E_t. E_p is the second transition energy (in addition to E_t) given by $E_g + E_p$. When the photon absorption energy is greater than E_p, the absorption is expressed as Lorentz linear absorption. E_u is the Urbach tail width, which is an important characterization parameter of material structure disorder and defect density. E_1 indicates that the imaginary part of the dielectric constant. ε_i is continuous at $E = Et$. $G(E)$ is a state density function approximated by a constant dipole. The real part of the dielectric constant ε_i can be obtained by Krames-Kronig transformation.

$$\varepsilon_r(E) = \varepsilon_\infty + \frac{2}{\pi}\boldsymbol{P}\int_0^\infty \frac{E'\varepsilon_2(E')}{E'^2 - E^2}dE' \tag{4}$$

The refractive index n and the extinction coefficient k can be calculated by the dielectric constant ε:

$$n = \sqrt{\frac{\sqrt{\varepsilon_r^2 + \varepsilon_i^2} + \varepsilon_r}{2}}, \quad k = \sqrt{\frac{\sqrt{\varepsilon_r^2 + \varepsilon_i^2} - \varepsilon_r}{2}} \tag{5}$$

The characteristics of transmittance spectra and reflectance spectra of the single coating-substrate are uniquely determined by the complex refractive index, the refractive index, the extinction coefficient and the physical thickness of the film. According to the theory of thin film optics, the reflectivity R^{Cal} and the transmittance T^{Cal} of the coating-substrate system can be calculated. By using the method of nonlinear constrained optimization, the optimal values of the refractive index, the extinction coefficient, and the physical thickness can be obtained by step-by-step iterations [12,13]. The imitative effect can be characterized by the evaluation function, as follows:

$$MSE = \sqrt{\frac{1}{2N}\sum_{j=1}^{N}\left[\left(\frac{T_j^{cal} - T_j^{\exp}}{\sigma_j^{cal}}\right)^2 + \left(\frac{R_j^{cal} - R_j^{\exp}}{\sigma_j^{cal}}\right)^2\right]} \tag{6}$$

Where $T_j^{\exp}$ is the measurements of the transmittance at the j_{th} wavelength, and Tcaljis the calculated value of the transmittance at the j_{th} wavelength. N is the number of data points measured, and $\sigma_j^{\exp}$ is the measurement error of the j_{th} wavelength transmittance.

3. Experiment and test

In our study, the germanium thin films were prepared by the electron beam evaporation technology using high-purity germanium on three kinds of substrates including double-sided polished ultra-smooth quartz, single-sided polished ultra-smooth quartz (Φ25 × 6 mm) and double-sided polishing of ZnS (Φ25 × 2 mm). The surface roughness of the substrate is better than 0.3 nm. The ZnS substrates were used for the measurement of the infrared spectrum. In this experiment, the low vacuum pump and the oil diffusion pump was adopted to ensure the standard vacuum. The substrate is heated to 180 °C and the surface of the substrate was cleaned for 5 min with a 16 cm ion source before the coating began. The deposition rate of germanium film was 0.3 nm/s, and the film thickness was monitored by IC5 crystal film thickness meter.

The spectral characteristics of the germanium film were measured using the lambda-900 spectrophotometer manufactured by PE, USA. Double-sided polished quartz samples were used to measure the transmission spectrum of the film, and the single-sided polished quartz samples were used to measure the reflectance spectrum of the film. The spectrum were scanned from 190 nm to 2600 nm at a speed of 50 nm/min. The measurement angle of the transmission spectrum and reflectance spectrum is 0° and 8° respectively. In addition, the Fourier transform spectrometer of PE company was used to test the spectrum from 1.25 μm to 15 μm. In order to obtain the optical constants of the germanium thin films from visible region to infrared region, the dielectric constant model of Eqs. (1)–(4) was use to fit the test spectra. Fig. 1 shows the transmission spectrum and the reflection spectrum in visible range of the germanium thin films based on the quartz substrate. Fig. 2 shows the transmission spectrum of the germanium thin films on the zinc sulfide substrate and the transmission spectrum of the ZnS substrate. The crystal structure characterization of the germanium thin films of the single-sided polished quartz substrate was carried out using D/max-2200 X-ray diffractometer with Cu K_a radiation of wavelength λ = 1.5405 Å and the filter is Ni. Other parameters include test voltage 40 kV, current 100 mA, scan speed 2°/min, scan angle 20°~80°, angle interval 0.1°, respectively. The X-ray diffraction pattern of germanium film is shown in Fig. 3.

From Fig. 1 it can be seen that the transmittance rapidly decrease to zero in the region less than 1 μm and there is a reflectance absorption peak appeared between 0.8 μm and 1 μm, but no obvious reflection extremum in the visible wavelength band, which indicated that the absorption coefficient of the film is larger in the visible range and could not form an effective reflection interference peak. In the long wavelength band of more than 1.25 μm, it is the transparent region of the germanium film, forming the interference transmission extreme peak which is shown in Fig. 2. In the X-ray diffraction spectrum, the diffracted peaks are in the vicinity of the diffraction angle of 20°, indicating that the film structure is amorphous. Therefore, the optical constants of the formulas (1)-(4) can be applied to the germanium thin films.

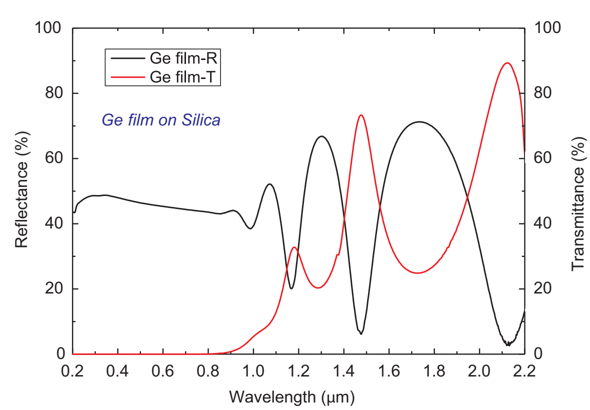

Fig. 1. The transmission spectrum and reflection spectrum in visible region of the germanium thin films of quartz substrate.