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Temperature dependence of the infrared optical constants of germanium films

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ABSTRACT

High-temperature transmittance spectrum of germanium films was obtained by a Fourier Transform infrared spectroscopy with a high-temperature accessory. The optical constants were determined by transmittance spectrum fitting with a Gaussian oscillator as the dispersion model. The analysis results showed that both the refractive index and extinction coefficient increased with the increasing temperature. The square of the refractive index increased linearly with the increasing temperature. The higher the temperature was, the faster the absorption coefficient increased. The germanium films were deposited on chemical vapor deposition ZnS substrates by ion-beam-assisted deposition. The region of temperature was between room temperature and 773 K, and the analysis spectrum was between 2000 nm and 5000 nm.

1. Introduction

Germanium is one of the most important high refractive index materials for optical coatings due to its wide transparent region in the infrared band. Germanium films could be fabricated by plasma-enhanced chemical vapor deposition [1,2],electron-beam evaporation [3–5], r.f.-magnetron sputtering [6,7], and laser deposition [8], etc. Ion-beam-assisted deposition (IBAD) has become one of the preferred methods to produce high-quality thin films [9], for its comparatively simple technic and improvement of mechanical and optical properties of the film approached by ion bombardment.

The optical constants of germanium films are determined by the deposition technique and parameters. Germanium films have been extensively researched on the optical and structural properties [5]. For the temperature dependent optical constants, some films have been reported, such as amorphous $Ge_2Sb_2Te_5$, silver and polycrystalline α-In_2Se_3 [10–12]. However, there is little discussion about temperature dependence of optical properties of germanium films.

In this article, the temperature-dependent optical constants of germanium films prepared by IBAD are analyzed with transmittance spectrum at different temperatures.

2. Experiments and calculating methods

2.1. Experiments

Germanium films were deposited on $\Phi 40 \times 5.5$ mm chemical vapor deposition (CVD) ZnS substrates, and the deposition equipment was equipped by a Kaufman ion source made by Veeco-Ion Technology. The diameter of the ion source is 16 mm, and the maximum power of the source is 600 W. The ion-source beam was directed off-center to the rotating substrate holder. The value of the ion-beam voltage, which determines the ion energy, was set 180 V. The ion-beam current was set 80 mA. The gas flow of argon (Ar) was kept at 22 sccm (standard-state cubic centimeter per minute) and 8 sccm for ion source and neutralization, respectively.

The precursor for evaporation was germanium slices with the purity 99.99%. Before the deposition, the substrates were pre-cleaned by Ar ion-beam bombardment for 5 min in order to further reduce contamination on the surface. During the deposition, the substrates were rotated at 20 rpm and the distance between the substrate and the evaporation source were 1300 mm.

The physical thickness of the films was designed about 1000 nm. The transmittance spectrum was measured by Fourier Transform infrared spectroscopy (FTIR) (PE Spectrum GX) with the high-temperature accessory. The spectrum region was from 5000 cm^{-1} to 2000 cm^{-1} with 1 cm^{-1} interval, while the aperture was 20 mm. 6 temperatures were set, which were RT (room temperature, 293 K) and from 373 K to 773 K with 100 K interval. The calefactive speed was 10 K per minute. After the temperature achieved the set value, the temperature kept

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10 min before the measurement. The transmittance spectrums at different temperatures of both the CVD ZnS substrate and the film were measured.

2.2. Calculating methods for optical constants

In this article, the optical constants of germanium films on different temperatures were calculated from transmittance spectrum in WVASE32 software. It is easy to use the GenOsc layer to combine a number of oscillators to model a layer's dielectric function. We choose Gaussian oscillators as GenOsc layer for germanium films. The Gaussian styles are as follows from function 1 to 4 [13].

$$\varepsilon_{n\_Gaussian} = \varepsilon_{n1} + i\varepsilon_{n2} \tag{1}$$

$$\varepsilon_{n2} = A'e^{-\left(\frac{E-E_n}{\sigma}\right)^2} - A'e^{-\left(\frac{E+E_n}{\sigma}\right)^2} \tag{2}$$

$$\sigma = \frac{Br_n}{2\sqrt{\ln(2)}} \tag{3}$$

$$\varepsilon_{n1} = \frac{2}{\pi} P \int_0^{\infty} \frac{\xi \varepsilon_{n2}(\xi)}{\xi^2 - E^2} d\xi \tag{4}$$

where, the $1/2\sqrt{\ln(2)}$ factor set the Broadening parameter $\mathrm{Br_n} =$ FWHM, $A' = \mathrm{A_n} / \mathrm{Br_n}$.

For the transmittance spectrum fitting, the evaluation function is important. We use the maximum likelihood estimator, which represents the quality of the match between the experimental data and calculated data. It should be positive and go to zero (or at least an absolute minimum) when the calculated data matches the experimental data exactly. The mean-squared error (MSE) is as follows [13]:

$$MSE = \sqrt{\frac{1}{2N-M} \sum_{i=1}^{N} \left(\frac{t_i^{\mathrm{mod}} - t_i^{\mathrm{exp}}}{\sigma_i^{\mathrm{exp}}} \right)^2} = \sqrt{\frac{1}{2N-M} \chi^2} \tag{5}$$

where N is the number of transmittance data, M is the number of variable parameters in the model, and σ are the standard deviations on the experimental data points. Another common maximum likelihood estimator, the chi-square (χ^2) is defined in Eq. (5) for comparison.

In the fitting process, the transmittance error was set 0.5% at every wavelength in the measure spectrum.

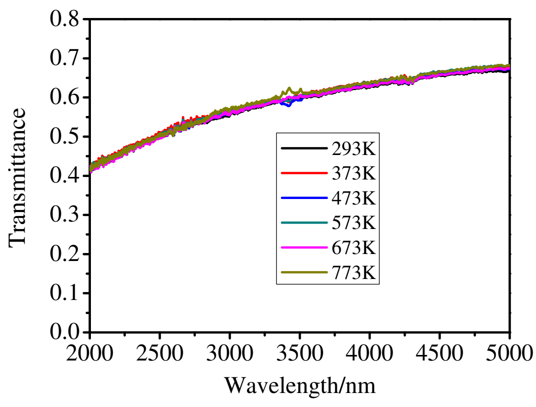

Fig. 1. Transmittance spectrum of CVD ZnS substrate at different temperatures.

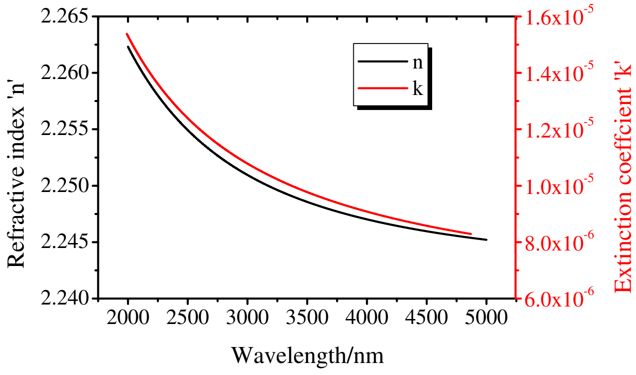

Fig. 2. Optical constants of CVD ZnS substrate.

3. Results and discussion

3.1. Optical constants of CVD ZnS substrate

Fig. 1 shows the transmittance spectrum of the CVD ZnS substrate at different temperatures. The transmittance almost does not change with the temperature, which is consistent with the results shown in Infrared Optical Materials [14]. So between 2000 nm and 5000 nm, we can consider that the optical constants are identical at all temperatures. Optical constants of CVD ZnS substrate are calculated by Cauchy dispersion model with Urbach absorption [13]. Fig. 2 shows the refractive index n and extinction coefficient k of CVD ZnS substrate, where k includes both the absorption and the scattering in the substrate.

3.2. Refractive index of germanium films

Fig. 3 shows the transmittance spectrum on different temperature of germanium film on CVD ZnS substrate. When the temperature is increasing, the peak transmittance decreases, and the transmittance peak position move toward longer wavelengths, which indicates that the optical thickness of germanium film increases with the increasing temperature.

The calculation results of refractive index of germanium films with transmittance spectrum are shown in Fig. 4. It can be seen that the refractive index increases with the increasing temperature at every wavelength in the analysis region.

With the results, the n^2 could be calculated, which is compared with the bulk germanium material given by temperature-dependent

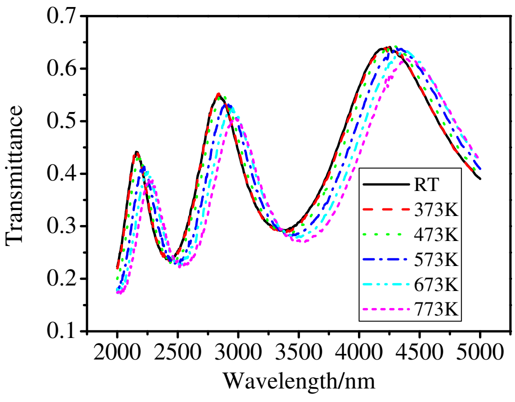

Fig. 3. Transmittance spectrum of germanium films on CVD ZnS substrate at different temperatures.