第 20 卷第 3 期
2001 年 6 月

红外与毫米波学报
J. Infrared Millim. Waves

Vol. 20, No. 3
June, 2001

REFRACTIVE INDEX ENHANCEMENT EFFECT IN $Hg_{1-x}Cd_xTe$ NEAR THE FUNDAMENTAL GAP*

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Abstract The refractive indices of $Hg_{1-x}Cd_xTe$ bulk samples with the composition $x=0.276$, 0.309, and 0.378 were measured by infrared spectroscopic ellipsometry at room temperature in the energy regions which were below, across, and above the fundamental band gap. An obvious refractive index enhancement effect was observed in the refractive index spectra for each composition. The energy position of the maximal refractive index value equals approximately that of the band gap. The refractive index versus wavelength λ above the band gap for x between $x=0.276$ and 0.378 was modeled using a Sellmeier dispersion relationship $n^2(\lambda)=a_1+a_2/\lambda^2+a_3/\lambda^4+a_4/\lambda^6$.

Key words infrared spectroscopic ellipsometry, refractive index, $Hg_{1-x}Cd_xTe$.

$Hg_{1-x}Cd_xTe$ 禁带宽度附近折射率增强效应*

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摘要 用红外椭圆偏振光谱测量了室温下 $Hg_{1-x}Cd_xTe$($x=0.276,0.309,0.378$)体材料位于禁带宽度之下、附近和之上的折射率. 对每一种组份样品均观察到明显的折射率增强效应. 折射率峰值所对应的能量位置近似等于其禁带宽度. 禁带宽度之上折射率随波长 λ 变化可用 Sellmeier 色散关系 $n^2(\lambda)=a_1+a_2/\lambda^2+a_3/\lambda^4+a_4/\lambda^6$ 进行拟合.

关键词 红外椭偏光谱，折射率，$Hg_{1-x}Cd_xTe$.

INTRODUCTION

The refractive index dispersion near the fundamental gap in semiconductors is significant for the design and analysis of the optoelectronic devices, such as optical filters, mirrors coated with thin films, semiconductor lasers and modulators. The refractive indices of bulk materials exhibit remarkable changes at the fundamental absorption edge, which has been investigated for Ⅲ-Ⅴ compounds[1] and narrow-gap lead salts[2]. This phenomenon has also been observed in MBE layers of $Pb_{1-x}Eu_xSe$, $Pb_{1-x}Sr_xSe$[3] and $Pb_{1-x}Eu_xTe$[4], as well as in two-dimensional $PbTe/Pb_{1-x}Eu_xTe$ MQW structures[5]. However, it is not observed in the narrow-gap semiconductor mercury cadmium telluride $Hg_{1-x}Cd_xTe$ (MCT), a very important material in infrared applicatoins.

The usual methods to determine the refractive indices of MCT are based on the transmission spectra of thin samples[6~10]. Unfortunately, only the refractive index below the band can be available by this technique, due to large absorption coefficients in MCT above the band gap. To describe the refractive indices near the band, in this paper we investigated the refractive indices of $Hg_{1-x}Cd_xTe$ bulk samples with the composition $x=0.276$, 0.309, and 0.378 in the energy region which are below, across and above the fundamental gap by infrared spectroscopic ellipsometry. An explicit refractive index enhancement effect was observed in MCT bulk material for each composition.

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* The project supported by the National Natural Science Foundation of China (No. 69738020)
Received 2000-08-16, revised 2000-12-13

* 国家自然科学基金(编号 69738020)资助项目
稿件收到日期 2000-08-16，修改稿收到日期 2000-12-13

1 EXPERIMENTAL

The samples were prepared by the Bridgman method, then annealed in Hg vapor to form n-type crystals (with carrier concentration $2-5\cdot10^{14}$ cm^{-3}). The transmission spectra of the samples were recorded using FTIR spectrometer (Bio-Rad Co. FTS-65A). The alloy compositions of the measured samples were determined by fitting the transmission spectra near the fundamental absorption edge with the empirical formulas of the energy gap and absorption rules[11~13].

The surfaces of $Hg_{1-x}Cd_xTe$ samples to be measured by infrared spectroscopic ellipsometry were mechanically polished. The back surfaces of the samples were roughed by silicon carbide sandpaper to suppress the component of the beam reflected from the back sides of the samples.

Spectroscopic ellipsometry meaures the complex reflectance ratio ρ between the reflection coefficients r_p and r_s, which are the light polarized parallel and perpendicular to the plane of incidece, respectively. By analyzing the state of the polarization of reflected light, one determines two parameters: tan ψ and cosΔ, which are related to ρ by

$$\rho=\frac{r_p}{r_s}=\tan\psi\exp(i\Delta), \tag{1}$$

The dielectric function $\varepsilon=\varepsilon_1+i\varepsilon_2$ of the sample can be calculated by using an ideal two-phase model[14]:

$$\varepsilon=\varepsilon_a\left[\sin^2\varphi_0+\sin^2\varphi_0\tan^2\varphi_0\left(\frac{1-\rho}{1+\rho}\right)^2\right]; \tag{2}$$

where ε_a is the dielectric function of a transparent ambient without regarding to the possible presence of overlayers, and φ_0 is the angle of incidence.

Then the refractive index and extinction coefficient are obtained as follows:

$$n=\frac{1}{\sqrt{2}}\sqrt{\sqrt{\varepsilon_1^2+\varepsilon_2^2}+\varepsilon_1},$$

$$k=\frac{1}{\sqrt{2}}\sqrt{\sqrt{\varepsilon_1^2+\varepsilon_2^2}-\varepsilon_1}. \tag{3}$$

The ellipaometric measurements were carried out by an automatic infrared spectroscopic ellipsometer, the polarizer and analyzer of which are synchronously rotat with a speed ratio of 1:1[15] at an angle of incidence 73°. The light source was a 1000W water-cooled globar lamp. The spectroscopic ellipsometric measurements were carried out in air over the energy range 0.1 ~ 0.5eV. The probe beam diameter size was $\varphi\approx$4mm. The absolute values of measured refractive index are accurate to 1% in the measurements without any defect correction for the instrumental elements, which is quite good for infrared spectroscopic ellipsometers.

2 RESULTS AND DISCUSSION

Fig. 1 shows the measured refractive indices n of the $Hg_{1-x}Cd_xTe$ bulk samples with $x=0.276$, 0.309, and 0.378 versus photon energy in the infrared region. We obtain the refractive indices not only below the band gap, but also across and above the energy gap for different compositions. As it is shown in the figure, a peak in the refractive index curve appears for each composition. The refractive index enhancement effect is obviously observed, which can be understood according to the following Kramers-Kronig (KK) analysis:

$$n(\nu)=1+\frac{c}{\pi}\int_0^{\infty}\frac{\mathrm{d}\alpha(\nu')}{\mathrm{d}\nu'}\log\frac{\nu'+\nu}{\nu'-\nu}\mathrm{d}\nu', \tag{4}$$

where ν', ν are frequencies, c is the light velocity, $\alpha(\nu')$ is the absorption coefficient at frequency ν'. As well-known, a complete intrinsic absorption spectrum includes not only the Urbach exponential-absorption edge but also the Kane region. The former results from the transitions other than band-to-band transitions, such as the transitions of electron-hole, electron-phonon, and electron-impurity and the latter is due the optical transitions of electrons from the valence band to the conduction band. They obey different absorption rules[16]. In the energy region near the absorption edge, the value of $\mathrm{d}\alpha(\nu')/\nu'$ goes up and the refractive index increases as the photon energy. However, when the photon energy reaches the gap energy, the absorption curve changes its slopes and becomes flatter, so the value of $\mathrm{d}\alpha(\nu')/\nu'$ decreases above the gap energy. Therefore, a peak appears

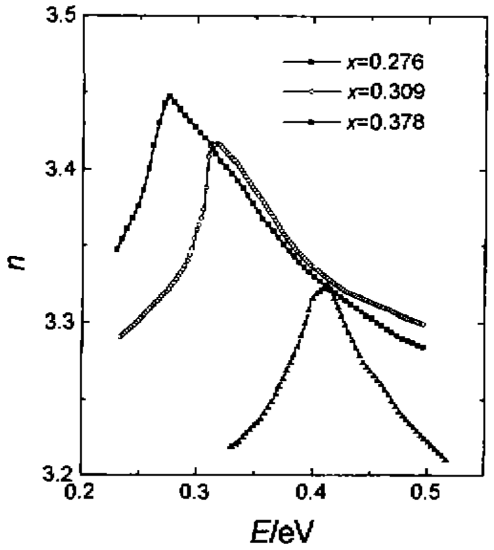

Fig. 1 The refractive indices n of the $Hg_{1-x}Cd_xTe$ bulk samples with $x=0.276, 0.309$, and 0.378 measured by infrared spectroscopic ellipsometry at the energies which are below, across, and above the band gap at room temperature

图 1 用红外椭偏仪测得的组分为 0.276，0.309 和 0.378 $Hg_{1-x}Cd_xTe$ 在禁带宽度能量之下、附近和之上的室温折射率 n

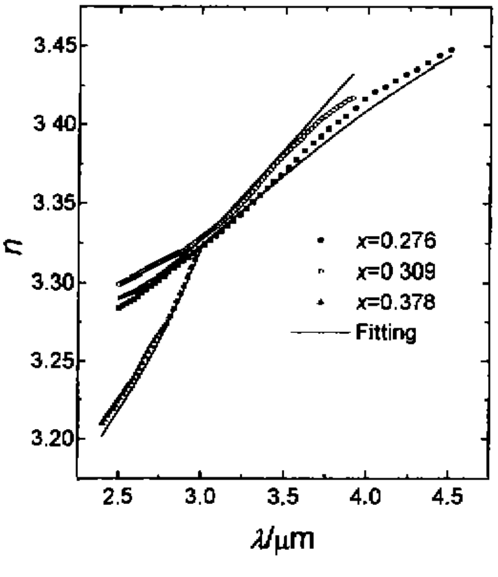

Fig. 2 Measured and fitting refractive index spectra versus wavelength above the band gap of $Hg_{1-x}Cd_xTe$ bulk samples with $x=0.276, 0.309$, and 0.378

图 2 不同组分 $Hg_{1-x}Cd_xTe$ 禁带宽度之上折射率实验数据及拟合曲线

in the refractive index curve at the band gap energy.

Furthermore, the peak will move toward the lower energy and its value will increase as the composition decreases. The refractive index above the band gap will drop quickly near the gap then decrease slowly as energy increases.

Thin overlayers, such as oxides and microscopic roughness on the sample surface, have effects on the optical constants. We found in our measurements that finite overlayers mainly affected the extinction coefficients. Therefore the refractive indices reported here are observed without including the correction made for possible surface overlayers or damage effects. Since the back sides of the samples were roughed, the reflcetion of the light beam from the back sides of the samples is very small and its contribution to n is less than 1% by estimation below the band gap. Therefore there is no correction to the values of the refractive indices below the band gap due to the back reflection contribution.

From the energy position of the refractive index peaks shown in Fig. 1, the band gap is about 0.275, 0.371, and 0.414eV, which is very near the value 0.273, 0.318, and 0.413eV obtained from the band gap formula[1,2] with the composition $x=0.276$, 0.309, and 0.378, respectively. A theoretical naalysis[7] showed that the near-to-gap $n(E)$ enhancement in narrow gap semiconductors was dependent on energy gap E_g, absorption edge steepness and brodening W_0. And Zemel[2] proposed that the position of the maximum was predicted at $E_g+W_0/2$ rather than at E_g. It shows that the impurity concentration in our samples is low enough that the broadening effect is negligible in the experimental errors.

Table 1 Fitting parameters of the refractive indices for $Hg_{1-x}Cd_xTe$ bulk samples with $0.276 \leqslant x \leqslant 0.378$ above the band gap at room temperature

表 1 室温下 $Hg_{1-x}Cd_xTe$ ($0.276 \leqslant x \leqslant 0.378$) 体样品在能量大于禁带宽度时折射率拟合参数

Coefficient	A_i	B_i	C
a_1	23.901	−108.977	253.281
a_2	−43.560	821.897	-2.627×10^3
a_3	-1.400×10^3	5.256×10^3	1.212×10^4
a_4	5.781×10^5	-2.828×10^4	2.392×10^4

Up to now there is no report on the refractive index spectra of MCT above the band gap. They are plotted separately in Fig. 2 as a function of wavelength λ (in micrometers). The best fit with experimental results at room temperature for x between $x = 0.276$ and 0.378 is obtained from the Sellmeier equation

$$n^2(\lambda) = a_1 + a_2/\lambda^2 + a_3/\lambda^4 + a_4/\lambda^5, \qquad (5)$$

where $a_i = A_i + B_i x + C_i x^2$ (i=1,2,3,4) and the coefficients A_i, B_i and C_i are given in table 1. The fitted refractive in dex spectra are presented in Fig. 2 by solid lines. The maximum difference between the experimental values and this formula is less than 0.5%, which is better than the experimental errors.

4 SUMMARY

In conclusion, we have measured the dispersion of the refractive indices of $Hg_{1-x}Cd_xTe$ ($x = 0.276$, 0.309, and 0.378) bulk samples at room temperature by infrared spectroscopic ellipsometry in the energy regions which are below, across, and above the fundamental band gap, respectively. An obvious refrative index enhancement effect is observed for each composition, which can be accounted for in accordance with KK relation. The energy of the band gap obtained from the refractive index peak is in good agreement with that from the band gap formula. The experimental values of the refractive indices above the band gap have been fitted well by a Sellmeier equation.

ACKNOWLEDGMENTS

The authors would like to acknowledge Prof. Guoshen Xu, Guoliang Shi for their helpful technique assistance.

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