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OPTICAL PROPERTIES OF $Zn_{1-x}Mg_xSe$ EPILAYERS STUDIED BY SPECTROSCOPY METHODS

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Linear optical properties of the $Zn_{1-x}Mg_xSe$ ($0 \leq x \leq 0.4$) alloys have been studied using reflectance, spectroscopic ellipsometry and photoluminescence measurements. The refractive indices of $Zn_{1-x}Mg_xSe$ epilayers were investigated as a function of Mg composition ($0 \leq x \leq 0.4$). The energies of band gap E_g and spin-orbit splitting $E_g + \Delta$, have been determined. These energies are shifted gradually to higher values with increasing Mg content.

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1. Introduction

Interest in mixed II–VI semiconductor materials arises because they can be made with preselected physical properties and hence have applications in various electronic and opto-electronic devices.

Knowledge of the band-gap energy value (E_g), linear (α) and nonlinear (β) absorption coefficients, refractive indices (n) and the third-order susceptibility ($\chi^{(3)}$) of the ternary and quaternary epilayers grown on different substrates is especially important for design and analysis of laser structures, as well as in waveguiding devices utilizing these semiconductors in the ultraviolet, visible, and infrared ranges [1].

Although the linear optical properties of ZnSe, ZnTe crystals and layers have been recently well established, still little is known about linear and nonlinear properties of their alloys.

In this work, we studied the linear optical properties of $Zn_{1-x}Mg_xSe$ epitaxial layers grown on GaAs using reflectance (REF), spectroscopic ellipsometry (SE) and photoluminescence (PL) methods.

2. Experimental

The $Zn_{1-x}Mg_xSe$ epilayers were grown on GaAs (001) and ZnTe (111) and silica glass substrates by solid source MBE in facility described elsewhere [2]. The photoluminescence and photoreflectivity spectra were measured in the temperature range from 10 to 300 K using a closed cycle cryogenic system (APD-Cryogenic Inc.). Low-temperature reflectance measurements have been performed in backscattering geometry using a 100 W tungsten-halogen lamp as a light source [3, 4].

3. Results

Figure 1 presents typical reflection (Fig. 1A) spectra of $Zn_{1-x}Mg_xSe$ epitaxial layers grown on GaAs substrate. The transmission spectra of $Zn_{1-x}Mg_xSe$ thin film, grown on silica glass in the same conditions, are shown in Fig. 1B. The strong interference fringes occur in the spectra for $h\nu \leq E_g$, where the epilayer is transparent and disappears abruptly for $h\nu > E_g$. The refractive indices of $Zn_{1-x}Mg_xSe$ epilayers were investigated as a function of Mg composition ($0 \leq x \leq 0.4$) and were deduced from interference fringes.

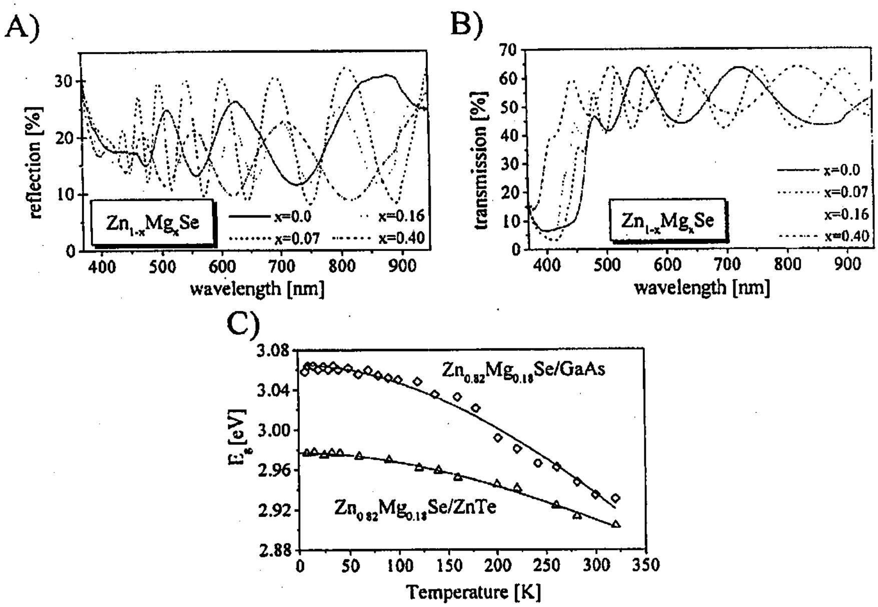

Fig. 1. Optical reflection (A) and transmission (B) spectra of $Zn_{1-x}Mg_xSe$ layers with the composition x indicated in the legend. The temperature dependence of band gap energy for $Zn_{1-x}Mg_xSe$ grown on GaAs and ZnTe substrates (C). The solid line represents the fit of the data to Varshni's expression (Eq. (1)).

The band-gap energies of all samples were estimated from measurements of reflection and transmission spectra near to the fundamental absorption edge at different temperatures [4, 5]. The temperature dependence of E_g for $Zn_{1-x}Mg_xSe$ epilayers grown on GaAs and ZnTe substrates has been estimated and is presented in Fig. 1C. The solid line represents the fit of the data to Varshni's expression [6]

$$E(T) = E_g(0) - \frac{\alpha T^2}{T+\beta}. \tag{1}$$

Based on the obtained data this formula may be expressed as

$$E(T) = 3.06 - \frac{0.00149T^2}{T+736.5} \tag{2}$$

for the $Zn_{0.82}Mg_{0.18}Se$ layer grown on GaAs, and

$$E(T) = 2.98 - \frac{0.00065T^2}{T+575.9} \tag{3}$$

for the $Zn_{0.82}Mg_{0.18}Se$ layer grown on ZnTe.

Because the band-gap energy and lattice constant of $Zn_{1-x}Mg_xSe$ increase with Mg content the biaxial compressive strain appears at the interface and causes an additional shift of the band-gap energy towards a higher photon energy. When $Zn_{1-x}Mg_xSe$ layer is grown on ZnTe substrate, we observe a shift of E_g (compared to $Zn_{1-x}Mg_xSe$/GaAs substrate) in opposite direction due to the presence of tensile strain. We observed the same behaviour in photoluminescence spectra. Moreover, the luminescence band of higher intensity in blue emission region is assiociated with radiative recombination of free excitons. At high temperatures (above 130–150 K) the free excitons recombination is thermally quenched and the low energy emission coming from the deep levels recombination is observed [2].

Using spectroscopic elipsometry dielectric functions and their derivative spectra can be determined and then the energies of band gap E_g ($\Gamma_8^v \rightarrow \Gamma_6^c$ transition) and their spin–orbit splitting $E_g + \Delta$ ($\Gamma_7^v \rightarrow \Gamma_6^c$ transition), may be calculated. These energies are shifted gradually to higher energies with the Mg content increase and have been determined as the peak position of the reflection spectra just after the interference oscillations as it is marked by arrows in Fig. 2A.

The values of the energies E_g and $E_g + \Delta$ are 2.707 eV and 3.133 eV for the $Zn_{0.95}Mg_{0.05}Se$ layer grown on GaAs and 2.697 eV and 3.123 eV for the layer grown on ZnTe, respectively. A variation of temperature from room temperature to 10 K resulted in a decrease in refractive index and in energy shift to higher energies of the absorption edge (about 120 meV) independent of the Mg content of the layer. Refractive indices of $Zn_{1-x}Mg_xSe$ epilayers with different Mg content x, as a function of the photon energy E_p, at room temperature are shown in Fig. 2B.

The results can be described using the modified single effective oscillator method [7]. In this method refractive index n can be expressed as a function of the oscillator energy (E_0), the dispersion energy (E_d), the photon energy (E_p) and the band-gap energy E_g by

$$n^2 - 1 = \frac{E_d}{E_0} + \frac{E_d E_p^2}{E_0^3} + \frac{E_d E_p^4}{2E_0^3(E_0^2 - E_g^2)} \ln\left(\frac{2E_0^2 - E_g^2 - E_p^2}{E_g^2 - E_p^2}\right). \tag{4}$$

The E_d, E_0, and E_g are estimated and they vary linearly as a function of average Mg content of the layers.

In this work the refractive indices were fitted to a one-pole Sellmeier equation of the form [8]

$$n^2(\lambda) = A + \frac{B\lambda^2}{\lambda^2 - C}. \tag{5}$$

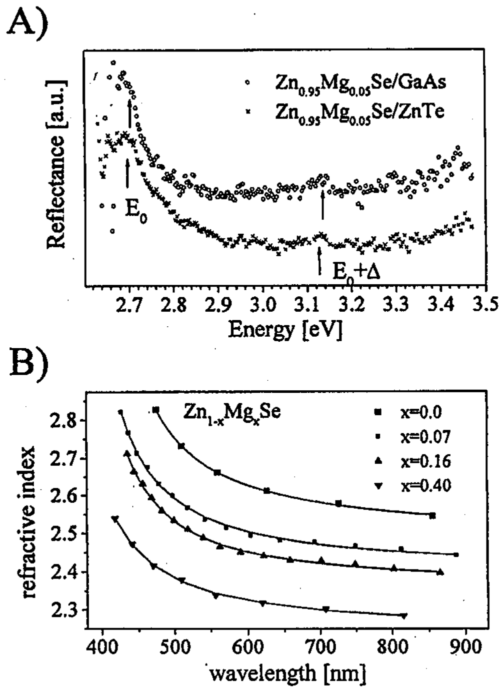

Fig. 2. Reflection spectra of $Zn_{1-x}Mg_xSe$ layers grown on GaAs and ZnTe substrate (A). The arrows indicate the energies of band gap ($\Gamma_8^v \rightarrow \Gamma_6^c$ transition) and their spin–orbit splitting ($\Gamma_7^v \rightarrow \Gamma_6^c$ transition). Dispersion relation of the refractive indices of $Zn_{1-x}Mg_xSe$ layers. The solid line represents the fit of the data to the Sellmeier relation (Eq. (5)).

The parameters used to fit the data for the $Zn_{1-x}Mg_xSe$ layers are given in Table. The behaviour of the parameters A, B and C, which depend on the Mg content x and temperature T, has been derived by fitting them with a parabolic dependence on the Mg content

$$A(x) = 5.255 - 0.0208x - 2.243 \times 10^{-5}x^2, \tag{6}$$

$$B(x) = 2.887 - 0.0865x + 1.66 \times 10^{-3}x^2, \tag{7}$$

$$C(x) = 1.423 - 0.00358x - 7.103 \times 10^{-5}x^2. \tag{8}$$

No significant improvement in the fit was obtained by the use of a more general five-parameter, two-pole equation [8].

Moreover, it is shown that the dependence of the refractive index on the Mg content and on the wavelength is well described by a Sellmeier relation. E_g and $E_g+\Delta$ energies are shifted gradually to higher energies as the Mg content increases, indicating the gradual increase in the band-gap energy of the $Zn_{1-x}Mg_xSe$ alloys.

All samples studied reveal a strong nonlinear absorption which decreases with an increase in Mg content in $Zn_{1-x}Mg_xSe$ layers [9].

TABLE

Parameters used to fit the data for $Zn_{1-x}Mg_xSe$ layers grown on GaAs substrate.

Mg concentration x	A	B	C
0 (ZnSe)	5.2920	0.9649	144948
0.07	5.0302	0.7823	133930
0.16	4.9646	0.6454	138161
0.40	4.3842	0.6916	116293

4. Conclusions

We have measured the refractive indices of $Zn_{1-x}Mg_xSe$ epilayers as a function of Mg concentration, temperature and photon energy. The refractive indices were fitted to a one-pole Sellmeier equation. Using the measured dielectric function (from spectroscopic ellipsometry measurements) and their second-derivative spectra, the energies of band gap E_g ($\Gamma_8^v \rightarrow \Gamma_6^c$ transition) and their spin-orbit splitting $E_g + \Delta$ ($\Gamma_7^v \rightarrow \Gamma_6^c$ transition), have been determined. These energies are shifted gradually to higher energies as the Mg content increases.

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