# Optical properties of Zn<sub>1-x</sub>Mg<sub>x</sub>Se epilayers studied by reflection spectroscopy\*

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Linear optical properties of the  $Zn_{1-x}Mg_xSe$  ( $0 \le x \le 0.4$ ) alloys have been studied using reflection spectroscopy. The refractive indices of  $Zn_{1-x}Mg_xSe$  epilayers were investigated as a function of Mg composition ( $0 \le x \le 0.4$ ). The Sellmeier law is applied to describe the refractive index behaviour as a function of wavelength and magnesium concentration.

**Keywords:** reflection spectroscopy, refractive index, A<sub>2</sub>B<sub>6</sub> compounds

#### 1. Introduction

Mixed ternary and quaternary alloys of wide-gap A<sub>2</sub>B<sub>6</sub> semiconductors are very attractive materials for optoelectronics applications [1]. The usefulness of these materials arises from the possibility of tuning of bandgap energies, lattice constants and optical properties by adjusting the content of particular elements. Precisely knowledge of band structure, dispersion of refractive index and absorption coefficient, thickness and surface roughness of Zn<sub>1-x</sub>Mg<sub>x</sub>Se layers grown on different substrates is especially important in design and analysis of optoelectronics devices working in wide wavelength range. Knowledge of the refractive indices and absorption coefficients of semiconductors is especially important in the design and analysis of heterostructure lasers as well as other waveguiding devices utilising these materials. Although the optical properties of ZnSe have been well established recently [2], little is known about their aloys.

In this article, we present a detailed investigation of the optical reflection indices of  $Zn_{1-x}Mg_xSe$  layers grown on different substrates in the composition range ( $0 \le x \le 0.4$ ). The refractive indices with various Mg compositions were evaluated from the reflectance measurements.

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## 2. Experimental

The ZnMgSe epilayers were grown on (001) oriented GaAs and (111)<sub>Zn</sub> oriented ZnTe substrates by solid source MBE in facility described in Ref. 3. The ZnMgSe layers with different content of Mg were deposited by MBE method onto glass substrates (Corning 7059) too. The film grown on the glass substrate was used as a reference for comparison purposes. The reflectivity spectra were measured in the temperature range from 10 to 300 K using a helium closed cycle cryogenic system (APD-Cryagenic Inc.) and a SPM-2 monochromator (Zeiss) with a photomultiplier R-375 (Hamamatsu). Reflectance measurements have been performed in backscattering geometry using a 100 W tungsten-halogen lamp as a light source [4,5]. Optical spectra were measured for a series of Zn<sub>1-x</sub>Mg<sub>x</sub>Se with different compositions. The Mg content in Zn<sub>1-x</sub>Mg<sub>x</sub>Se layers was determined from X-ray diffraction measurements assuming a linear dependence of the lattice constant with Mg concentration. The obtained reflectance measurement was assumed to be equivalent to the case of normal incidence.

#### 3. Results and discussions

A typical reflectivity spectra are displayed in Fig. 1(a) for  $\rm Zn_{1-x}Mg_xSe$  layers deposited on GaAs substrate. Interference effects of the beams reflected at the two interfaces (air/epilayer and epilayer/substrate)

give rise to oscillations of the reflected intensity. For comparison we show in Fig. 1(b) transmission spectra of  $Zn_{1-x}Mg_xSe$  thin films, grown on silica glass in the same conditions and Mg composition. The spacing between adjacent fringes depends on the optical thickness of the layer ( $I_0 = nd$ ). The band gap energy of the  $Zn_{1-x}Mg_xSe$  layer corresponds to the limit of the last interference fringe. The temperature dependence of the band gap energies for  $Zn_{1-x}Mg_xSe$  epilayers grown on GaAs and ZnTe substrates has been estimated from reflection spectra. Behaviour of this phenomenon may be described by the Varhni's expression [6]

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

From the best fit to this formula we obtained the energy band gap  $E_g$  for the temperature T=0~K,  $\alpha$  and  $\beta$  parameters: 3.06 eV, 0.0015, and 736.5 for  $Zn_{0.82}Mg_{0.18}Se$  layer grown on GaAs and 2.98 eV, 0.00065 and 575.9 for  $Zn_{0.82}Mg_{0.18}Se$  layer grown on ZnTe, respectively.

The refractive indices of  $Zn_{1-x}Mg_xSe$  epilayers were deduced as a function of Mg composition  $(0 \le x \le 0.4)$ . The refraction index n, was obtained from examination of the interference fringe minima and maxima in reflection to determine their order

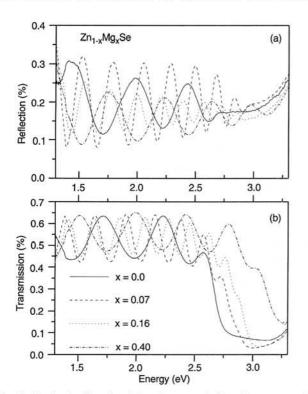


Fig. 1. Optical reflection (a) and transmission (b) spectra of  $Zn_{1-x}Mg_xSe$  layers with magnesium content indicated in the legend.

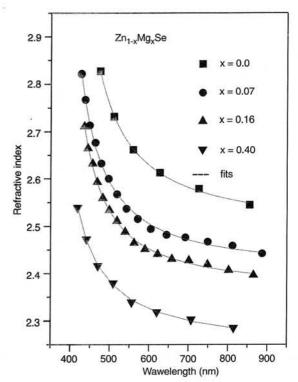


Fig. 2. Refractive index dispersion in  $Zn_{1-x}Mg_xSe$  alloy with different x composition.

numbers m. Then  $n = m\lambda_m/2d$ , where  $\lambda_m$  is the wavelength at the  $m^{th}$  extremum and d is the thickness. Since m is a small integer, it could be determined without error. The uncertainty in the value of  $\lambda_m$  is so much smaller than the error in d, which we estimate at  $\pm 4\%$ , that the error in n may be taken as equal to the error in d. Thickness value of  $Zn_{1-x}Mg_xSe$  layers was obtained from envelopes of interference fringes in transparent region of spectra, far from absorption edge. Refractive indices of  $Zn_{1-x}Mg_xSe$  epilayers with the different magnesium content x, as a function of the photon energy E, at room temperature are shown in Fig. 2.

Generally, the dispersion of the refractive index for many materials is fit to the first order Sellmeier's formula [7]

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

where A, B and C are the resulting curve-fitting parameters, and have no special physical significance. The variations of the Sellmeier parameters with alloy compositions are presented in Fig. 3 and fitting them with a parabolic dependence on the Mg content are derived as below

 $A(x) = 5.255 - 0.0207x - 0.0000224x^2$ 

 $B(x) = 0.964 - 0.0288x + 0.00055x^2$ 

 $C(x) = 142361 - 358x - 7.103x^2$ 

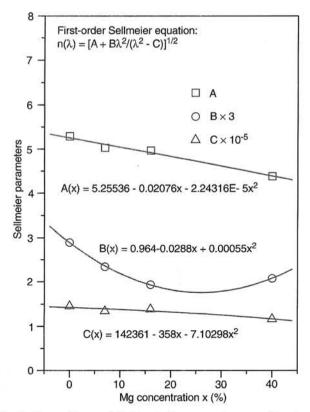


Fig. 3. Dependence of Sellmeier's parameters as a function of magnesium content x.

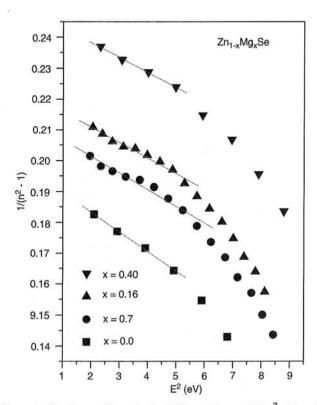


Fig. 4. Reciprocal polarizability  $1/\chi = 1/(n^2-1)$  of  $Zn_xMg_xSe$  layers plotted vs  $E^2$ . Solid lines are the best single effective oscillator fit.

These relations clearly show the complex dependence of the refractive index on alloy composition. The comparison of the refractive index values obtained by this method to the results from ellipsometry measurements at 632.8 nm gives good accuracy.

Wemple and DiDomenico [7,8] have proposed a single-effective-oscillator model which describe the refractive index data as a function of photon energy for a wide variety of materials at energies sufficiently below the direct band edge. The solid lines in Fig. 4 show the best fit of the single-effective-oscillator formula

$$n^2 - 1 = \frac{E_0 E_d}{E_0^2 - E^2} \tag{3}$$

where E is the photon energy and  $E_0$  is the energy position parameter. These fit lines give the reciprocal of the polarizability  $\chi^{-1} = (n^2-1)^{-1}$  vs photon energy E, which from equation (3) is a straight line.

Dispersion of refractive index in the transparency region can be approximated by the modified single effective oscillator (MSEO) [9]. In this method, the refractive index n can be expressed as a function of the dispersion energy  $E_{\text{d}}$ , the oscillator energy  $E_{\text{0}}$ , the photon energy  $E_{\text{p}}$ , and the direct band gap energy  $E_{\text{T}}$  by

$$n(E) = \frac{E_d}{E_o} + \frac{E_d E_p^2}{E_o^3} + \frac{E_d E_p^4}{2E_o^3 (E_o^2 - E_r^2)} \ln \left( \frac{2E_o^2 - E_r^2 - E_p^2}{E_r^2 - E_p^2} \right)$$
(4)

However, the fit obtained by using this formula and using three-term Sellmeier equation [10] is not significantly better.

Since the first order Sellmeier coefficients A, B and C have been specified as a function of the alloy composition x, we can easily calculate the refractive index of  $Zn_{1-x}Mg_xSe$  alloys with the arbitrary composition x and the wavelength. The calculated refractive index as a function of the phonon energy E with magnesium concentration increments of 0.05 is shown in Fig. 5.

Figure 6 shows dependence of the refractive index n at  $\lambda = 470$ , 510, 560, 650 and 810 nm of  $Zn_{1-x}Mg_xSe$  on its band gap energy  $E_g$ . There is no strict reason for the linear dependence of  $n(\lambda)$  on  $E_g$ , but it will be the first approximation useful in understanding a general behaviour of  $n(\lambda)$ . Most of II–VI semiconductor alloys show that the bigger energy band gap  $E_g$  material has a smaller value of the refractive index n. As it can be seen in Fig. 6, measured samples  $Zn_{1-x}Mg_xSe$  also show such usual behaviour.

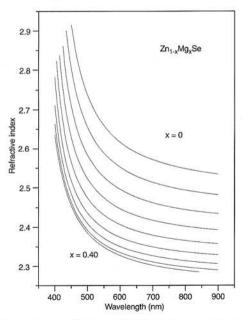


Fig. 5. Calculated refractive indices of  $Zn_{1-x}Mg_xSe$  layers with Mg concentration increment of 0.05.



The reflection spectroscopy are helpful contactless method for characterisation of  $Zn_{1-x}Mg_xSe$  layers. We have obtained Varhni's parameters and dispersion relation of the refractive indices  $n(\lambda)$  of  $Zn_{1-x}Mg_xSe$  layers. The dependence of  $n(\lambda)$  at fixed on  $E_g$  has been deduced. These results give fundamental parameters for optimum design of  $Zn_{1-x}Mg_xSe$  optoelectronics devices.

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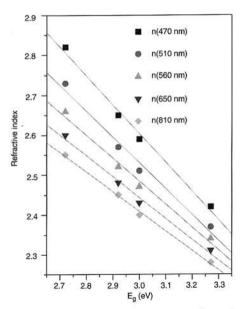


Fig. 6. Band gap energy dependencies of  $n(\lambda)$  at  $\lambda = 470$ , 510, 560, 650 and 810 nm.

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