Journal of the Korean Vacuum Science & Technology; JKVST
Vol.6, No.4, 2002, pp.149 ~ 152

Parametric modeling for the dielectric function of $Cd_{0.77}Mg_{0.23}Te$ alloy film

Yong-Sub Ihn, Tae-Jung Kim, and Young-Dong Kim†

Department of Physics and Basic Science Research Center, Kyung Hee University, Seoul 130-701, Korea

(Received December 2, 2002)

Abstract

We performed the modeling of the dielectric functions of $Cd_{0.77}Mg_{0.23}Te$ by using parametric semiconductor model. Parametric model describes the analytic dielectric function as the summation of several energy-bounded Gaussian-broadened polynomials and provides a reasonably well parameterized function which can accurately reproduce the optical constants of semiconductor materials. We obtained the values of fitting parameters of the Mg composition 0.23 in the parametric model. From these parameters we could remove interference oscillations to obtain the dielectric function of $Cd_{0.77}Mg_{0.23}Te$ alloy film for full 0.5 - 6.0 eV energy range.

1. Introduction

$Cd_{1-x}Mg_xTe$ alloys and related heterostructures have received much attention as a result of their high potential for optoelectronic devices [1]. Even though the properties of the binary endpoint CdTe of these alloys are well known [2,3], only a few studies of the critical point (CP) energies of CdMgTe alloys have been reported so far [4-6]. Since a knowledge of the optical response over a wide range of energy is of great importance for device applications, we performed the modeling of the dielectric function of $Cd_{0.77}Mg_{0.23}Te$ by using the parametric semiconductor model from 0.5 to 6.0 eV. We could remove interference oscillation pattern below E_0 edge to get the useful dielectric function value in the extended far infrared region.

2. Experimental

$Cd_{0.77}Mg_{0.23}Te$ alloy film was grown on [001] GaAs substrate by a molecular beam epitaxy. 3 μm thick $Cd_{0.77}Mg_{0.23}Te$ layer was grown, and had no cap layer of the surface. During CdMgTe deposition the surface showed a streaky reflection high energy electron diffraction (RHEED) pattern, and the composition of the layer was determined by high-resolution X-ray diffraction.

Pseudodielectric function spectra $\langle \varepsilon(\omega) \rangle = \langle \varepsilon_1(\omega) \rangle + i \langle \varepsilon_2(\omega) \rangle$ were measured at room temperature from 1.5 to 6.0 eV using an automatic spectroscopic rotating-analyzer ellipsometer (RAE) [7]. It is well known that the existence of overlayers on surfaces complicates efforts to obtain pure dielectric response ε because of its surface sensitivity [7]. Therefore, samples must be maintained in an inert atmosphere and etched in-situ immediately before measurement. We determined the effect of chemical reagents by flowing them over the vertical surface of an optically prealigned sample, rinsing the surface with the diluent(usually deionized water or methanol), then measuring the $\langle \varepsilon_2 \rangle$ spectrum [6]. The chemical treatment was repeated until the $\langle \varepsilon_2 \rangle$ spectra showed no further changes and the highest values of $\langle \varepsilon_2 \rangle$ in the E_2 CP region were obtained.

† E-mail : ydkim@khu.ac.kr

3. Results and Discussions

The measured real and imaginary parts of the pseudodielectric functions of $Cd_{0.77}Mg_{0.23}Te$ alloy film are shown in Fig. 1. The E_0+Δ_0, E_1, E_1+Δ_1, and E_2 structures are easily shown. However, we cannot obtain the accurate E_0 bandgap energy and dielectric function below the E_0 bandgap energy because of oscillation patterns. This oscillations at low energy result from interference involving the reflected component of the GaAs substrates, since the $Cd_{0.77}Mg_{0.23}Te$ alloy film is transparent in this energy region.

To remove the interference patterns, we performed the modeling of the dielectric functions of $Cd_{0.77}Mg_{0.23}Te$ by using the parametric semiconductor model [8]. This model describes the analytic dielectric function as the summation of several energy-bounded Gaussian-broadened polynomials and poles accounting for index effects due to absorption outside the model region. This model provides a reasonably well parametrized function which can accurately reproduce the optical constants of CdMgTe materials. This model begins with the treatment used to derive the Kim and Garland parametric dispersion model [9] and most other oscillator type dispersion models [10]. In this parametric model, the complex dielectric function is defined as a function of the photon energy E as,

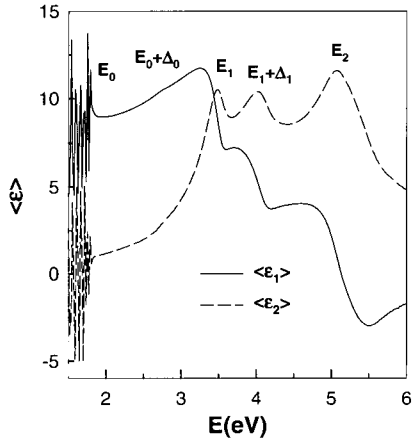

Fig. 1. Real(solid line) and imaginary(dashed line) parts of the pseudodielectric function of $Cd_{0.77}Mg_{0.23}Te$ at room temperature.

$$\varepsilon(E) = 1 + i\int_0^\infty W(E')\,\Phi(E, E')\,dE' \tag{1}$$

The variable E' is a dummy integration variable. The joint density of states is included in $W(E)$, the unbroadened absorption spectrum. The broadening function Φ is typically either Lorentzian or Gaussian, where the Kramers-Kronig consistency is built into

$$\Phi(E, E') = \int_0^\infty e^{i(E-E'+i\gamma(s))s}ds - \int_0^\infty e^{i(E+E'+i\gamma(s))s}ds \tag{2}$$

$\gamma(s) = \Gamma$ for Lorentzian broadening,

$\gamma(s) = 2\sigma^2\, s$ for Gaussian broadening.

The Eq. (1) comes to be

$$\varepsilon(E) = 1 + i\sum_{j=1}^{m}\int_{E_{\min}}^{E_{\max}} W_j(E')\,\Phi(E, E', \sigma_j)\,dE' + \sum_{j=m+1}^{m+P+1}\frac{A_j}{E^2 - E_j^2} \tag{3}$$

Eq. (3) is derived from Eq. (1) to represent the finite extent for which data is available by restricting the integration range and adding zero-width oscillators. The $W(E)$ function is broken into pieces which have an associated constant broadening parameter as below,

$$\begin{aligned}\Phi(\eta\omega, E, \sigma_j) &= \int_0^\infty e^{i(\eta\omega - E + i2\sigma^2 s)s}ds - \int_0^\infty e^{i(\eta\omega + E + i2\sigma^2 s)s}ds \\ &= \sqrt{\frac{\pi}{8\sigma^2}}\left[e^{-y_1^2} + e^{-y_1^2}\,\mathrm{erf}(iy_2) - e^{-y_2^2}\,\mathrm{erf}(iy_2)\right]\end{aligned} \tag{4a}$$

$$y_1 = \frac{\eta\omega - E}{2\sqrt{2}\sigma} \quad \text{and} \quad y_2 = \frac{\eta\omega + E}{2\sqrt{2}\sigma} \tag{4b}$$

$$W_j(E) = \sum_{k=0}^{N} P_{j,k}E^k\,u(E - a_j)\,u(b_j - E) \tag{4c}$$

where, the polynomials are grouped into four polynomial ensembles with 4th order polynomials (N=4 in

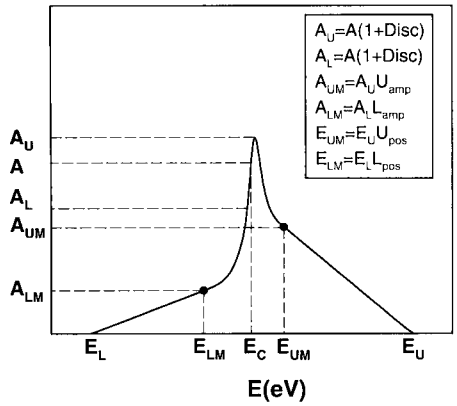

Fig. 2. A single CP structure described by the parametric model with four polynomial ensembles.

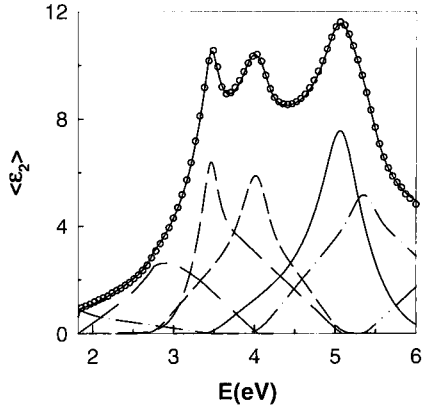

Fig. 3. Parametric model fit to dielectric function of $Cd_{0.77}Mg_{0.23}Te$ alloy with seven component critical point structures.

Eq. (4)), which are centered on critical point structures with the overlapping tails of adjacent ensembles filling in the intervening absorption regions, as depicted in Fig. 2. The center energies E_c correspond to the CP energies, while the bounding energies E_L and E_U delineate adjacent CPs. The positions of the two control points E_{LM} and E_{UM}, which correspond to the joining points of the four polynomials, are defined relative to these CP energies via relations in Eq. (4b). At the E_C discontinuities in amplitude and energy are permitted; hence the two sides of the ensemble are independent and step-like absorption features can be created to model direct bandgaps. The broadening parameter is primarily a local property at the CP energy and between CPs there is little sensitivity to the broadening. Each component of the model is like an oscillator, but the underlying delta function has been generalized to become a polynomial background, centered at an energy with amplitude and broadening parameter.

Figure 3 shows how the component CP structures combine to generate the $Cd_{0.77}Mg_{0.23}Te$ $<\varepsilon_2>$ spectra and the comparison of experimental data with our model dielectric function. The solid circles represent the experimental data for the imaginary part of $Cd_{0.77}Mg_{0.23}Te$, and the solid line represents the parametric model fit for the imaginary part. To clearly show the quality of the fits, the number of data points in the plot was reduced by half. The values of the parametric model for $Cd_{0.77}Mg_{0.23}Te$ are listed in Table 1. The defining parameters for a CP structure are as follows: center energy (E_c), center amplitude (A), broadening (B), upper and lower mid-positions (U_{mid}, L_{mid}), upper and lower mid-amplitudes (U_{amp}, L_{amp}).

Table 1. The parameter values for $Cd_{0.77}Mg_{0.23}Te$.

No	E	A	B	L_{mid}	L_{amp}	U_{mid}	U_{amp}
#0	1.8149	0.9291	23.355	0.5843	0.4089	0.6249	0.4930
#1	2.7769	2.5244	10.970	0.2170	0.1764	0.2399	0.3410
#2	3.4675	7.1725	43.405	0.3829	0.0052	0.7763	0.4956
#3	4.0395	7.4261	103.586	0.4987	0.2961	0.6775	0.0.3983
#4	5.0676	8.8876	105.312	0.2681	0.1147	0.1938	0.0024
#5	5.3710	6.9153	124.927	0.7750	0.5466	0.9020	0.6062
#6	7.0306	3.2359	44.123	0.4025	0.5660	0.5000	0.5969

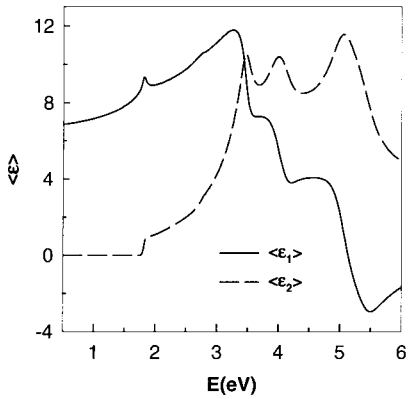

Fig. 4. The reconstructed dielectric function of $Cd_{0.77}Mg_{0.23}Te$ by the parametric semiconductor model.

Figure 4 shows that the real and imaginary parts of the dielectric function of $Cd_{0.77}Mg_{0.23}Te$ alloy film was obtained by the parametric semiconductor model. The solid and dashed lines represent data for the real and imaginary parts, respectively. All fine bandgap energies are clearly observed, and the dielectric function is extended beyond the experimentally available region for device applications, especially far infra-red range.

Ⅳ. Conclusions

We could obtain the pure dielectric function of $Cd_{0.77}Mg_{0.23}Te$ alloy film, using the chemical etching treatment. By using parametric semiconductor model, we could accurately reproduce the optical constants of $Cd_{0.77}Mg_{0.23}Te$ alloy film in far infrared region where the current experimental data are not available. We report the parameter values to reconstruct dielectric functions over wide energy range, so that those values can be used in designing optoelectronic devices with CdMgTe materials.

Acknowledgments

This work was supported by the National Research Laboratory Fund through Compound Semiconductor Epitaxy Laboratory (CSEL).

References

[1] A. Waag, H. Heinke, S. Scholl, C. R. Becker, and G. Landwehr, J. Cryst. Growth. **131**, 607 (1993).

[2] H. Arwin and D. E. Aspnes, J. Vac. Sci. Technol. A **2**, 1316 (1984).

[3] L. Vina, C. Umbach, M. Cardona, and L. Vodopyanov, Phys. Rev. B **29**, 6752 (1984).

[4] S. G. Choi, Y. D. Kim, S. D. Yoo, D. E. Aspnes, I. Miotkowski, and A. K. Ramdas, Appl. Phys. Lett. **71** (2), 14 (1997).

[5] M. S. Koo, M. S. Lee, T. J. Kim, Y. D. Kim, and I. K. Park, J. Korean Vac. Soc. **9** (3), 254 (2000).

[6] T. J. Kim, Y. D. Kim, S. D. Yoo, D. E. Aspnes, and J. Kossut, J. Korean Phys. Soc. **34**, 496 (1999).

[7] D. E. Aspnes and A. A. Studna, Appl. Opt. **14**, 220 (1975).

[8] B. Johs, C. M. Herzinger, J. H. Dinan, A. Cornfield, and J. D. Benson, Thin Solid Films. **313**, 137 (1998).

[9] C. C. Kim, J. W. Garland, and P. M. Raccah, Phys. Rev. B. **47**, 1876 (1993).

[10] H. D. Yao, P. G. Snyder, and J. A. Woollam, J. Appl. Phys. **70**, 3261 (1991).