Parametrization of the Optical Constants of $\text{AlAs}_x\text{Sb}_{1-x}$ Alloys in the Range 0.74-6.0 eV

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We report parameters that allow the dielectric functions $\varepsilon = \varepsilon_1 + i\varepsilon_2$ of $\text{AlAs}_x\text{Sb}_{1-x}$ alloys to be calculated analytically over the entire composition range $0 \leq x \leq 1$ in the spectral energy range from 0.74 to 6.0 eV by using the dielectric function parametric model (DFPM). The ε spectra were obtained previously by spectroscopic ellipsometry for $x = 0, 0.119, 0.288, 0.681, 0.829$, and 1. The ε data are successfully reconstructed and parameterized by six polynomials in excellent agreement with the data. We can determine ε as a continuous function of As composition and energy over the ranges given above, and ε can be converted to complex refractive indices using a simple relationship. We expect these results to be useful for the design of optoelectronic devices and also for *in situ* monitoring of AlAsSb film growth.

Keywords : AlAsSb , Dielectric function parametric model, Ellipsometry

OCIS codes : (120.2130) Ellipsometry and polarimetry; (160.6000) Semiconductor materials; (160.4760) Optical properties

I. INTRODUCTION

AlAsSb -based systems have been widely investigated for high-speed optoelectronic device applications such as ultrafast cross-phase modulators [1], quantum-cascade lasers [2], distributed Bragg reflectors [3], ultrafast all-optical switches using intersubband transitions [4], and photodetectors [5, 6]. The optical properties such as complex refractive index $\tilde{n} = n + ik$, dielectric function $\varepsilon = \tilde{n}^2 = \varepsilon_1 + i\varepsilon_2$, and interband transitions including the band gap of AlAsSb are needed for further device optimization [7], such as designs for distributed feedback grating waveguides [4] and simulations to predict the performance of solar cells [8, 9]. As a result, the dielectric functions and critical point (CP) energies of $\text{AlAs}_x\text{Sb}_{1-x}$ have been investigated using spectroscopic ellipsometry (SE) [10, 11], which is an excellent technique for determining ε data directly [12, 13]. However, no analytic representation of these ε spectra as a continuous function of As-composition x has been reported to date.

Here we analytically determine ε of $\text{AlAs}_x\text{Sb}_{1-x}$ as a continuous function of x for $0 \leq x \leq 1$ in the energy range from 0.74 to 6 eV. The source data were obtained previously by rotating-compensator SE [11]. In short,

pseudodielectric function $\langle \varepsilon \rangle$ spectra of $\text{AlAs}_x\text{Sb}_{1-x}$ alloy films (of well beyond the critical thickness to have bulk optical properties) with $x = 0.119, 0.288, 0.681$, and 0.829 were obtained on semi-insulating (001) GaAs substrates using molecular beam epitaxy (MBE). We performed *in situ* measurements directly on films grown by MBE, where the films were prepared and maintained in ultrahigh vacuum, preventing rapid oxidization of Al and ensuring oxide-free data. The endpoint data for AlAs and AlSb were taken from Refs. [14] and [15], respectively.

The CPs generate asymmetric features in ε [16]. Therefore, symmetric-lineshape models such as Lorentz, harmonic, or Gaussian oscillators provide poor representations of ε , requiring additional CP oscillators that have no physical basis. We circumvent this difficulty through the use of the dielectric function parametric model (DFPM) [17, 18], which can treat asymmetric characteristics appropriately while avoiding unnecessary additions. Here, we determine the parameters needed to represent ε analytically for the available spectra, then interpolate these parameters as a function of As composition x .

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II. MODELING

The DFPM has the advantage of properly representing ε data. In brief, in the DFPM the dielectric function is given as the sum of m energy-bounded polynomials that represent CP contributions within the accessible spectral range plus P poles that represent outside contributions [17, 18]. The general expression is

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

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

where

$$\Phi(\hbar\omega, E, \sigma_j) = \int_0^\infty e^{i(\hbar\omega - E + i2\sigma_j^2)s} ds - \int_0^\infty e^{i(\hbar\omega + E + i2\sigma_j^2)s} ds$$

$$= \sqrt{\frac{\pi}{8\sigma_j^2}} [e^{-y_1^2} + e^{-y_2^2} \operatorname{erf}(iy_1) - e^{-y_1^2} - e^{-y_2^2} \operatorname{erf}(iy_2)], \quad (2a)$$

$$y_1 = \frac{\hbar\omega - E}{2\sqrt{2}\sigma_j} \quad \text{and} \quad y_2 = \frac{\hbar\omega + E}{2\sqrt{2}\sigma_j}, \quad (2b)$$

$$W_j(E) = \sum_{k=0}^N P_{j,k} E^k u(E - a_j) u(b_j - E), \quad (2c)$$

where $u(x)$ is the unit step function. The use of pure Gaussian broadening in Eq. (2a) essentially prohibits closed-form integration of Eq. (1). However, the equivalent expression shown in Eq. (2b) shows that one-dimensional lookup tables as a function of $(\hbar\omega + E)/(2\sqrt{2}\sigma)$ can be constructed numerically for each order of polynomial required by Eq. (2c). The corresponding real part of ε is obtained by a Kramers-Kronig transformation. Detailed information, including a program to calculate the DFPM, is given in Refs. [17] and [18].

III. RESULTS AND DISCUSSION

We parameterized the ε spectra of $\text{AlAs}_x\text{Sb}_{1-x}$ alloy using

DFPM with $x = 0$ (AlSb), 0.119, 0.288, 0.681, 0.829, and 1 (AlAs). The source data for ternary alloys are obtained from our previous report [11], while data for AlAs and AlSb were taken from Refs. [14] and [15], respectively.

FIG. 1. (a) Dielectric function (open dots) of AlSb, together with the DFPM reconstruction (solid line) using six CP components (dashed lines). (b) Schematic of a single CP structure of E_1 in the DFPM.

TABLE 1. DFPM parameters for AlSb. Parameters denoted by asterisks are assumed to be independent of composition

CP	No.	E_L	E_U	E_C (eV)	A	B (meV)	E_{LM}	A_{LM}	E_{UM}	A_{UM}
E_0 (indirect)	0			1.603						
E_0 (direct)	1	0	2	2.19	0.3*	10*	0.6*	0.599	0.5*	0.8*
E_1	2	1	4	2.851	19.061	53.497	0.42*	0.084	0.8*	0.6*
$E_1 + \Delta_1$	3	1	4	3.226	20.051	119.844	0.7*	0.03*	0.8*	0.367
E_0'	4	3	6	3.777	59.790	302.243	0.7*	0.1*	0.423	0.08*
E_2	5	3	6	4.114	23.874	126.788	0.8*	0.2*	0.71*	0.06*
E_1'	6	4	7	5.2	7.047	213.087	0.2*	0.15*	0.8*	0.371
	7			15*						

As an example, Fig. 1(a) shows how the component CP structures combine to generate the ϵ_2 spectrum of AlSb. The open dots are the data from Ref. [15] while the solid line is the fit of the DFPM to these data. The dashed lines show the contributions of the six individual CPs. To show the quality of the fits better, we reduced the number of data points appropriately. The parameters obtained from Fig. 1(a) are listed in Table 1. In the present work each CP is described by nine parameters, which are depicted in Fig. 1(b). This is the ϵ_2 spectrum of the E_1 CP component of AlSb. Using the conventional names of the DFPM, E_C is the CP energy, while the values E_L and E_U indicate the CP structure numbers whose CP energies (E_C) are the lower and upper bounding energies, respectively. E_{LM} and E_{UM} are control points for establishing the asymmetric characteristics of the lineshape. The values E_{LM} and E_{UM} are not absolute energies but rather relative positions between E_L and E_C and between E_U and E_C , respectively. A_{LM} , A , and A_{UM} are the respective amplitudes at E_{LM} , E_C , and E_{UM} . Also, the values A_{LM} and A_{UM} are amplitudes relative to A . Parameter B , not shown in Fig. 1(b), is the full-width-half-maximum broadening parameter inherently embedded in harmonic-oscillator lineshapes. To construct the lineshape of a CP, second- and fourth-order polynomials were used for the energy regions (I, IV) and (II, III), respectively, with the constraint that the lines are connected smoothly and the values forced to zero at the boundaries E_L and E_U . Parameters that are held constant independent of composition are indicated by asterisks in Table 1. Here, No. 0 (E_0 indirect) and No. 7 are not CPs but are the lower bounding energy of E_0 (direct) and upper bounding energy of E_1' , respectively. The analysis was repeated for all AlAsSb spectra, and the fitting quality was similar to that seen for AlSb.

The reported $\langle\epsilon\rangle$ spectra of ternary alloys have oscillations below the E_0 feature, which are interference effects involving light back-reflected at the substrate-film interface, as a result of the films being transparent below their fundamental absorption edges. To extract ϵ in the oscillation region we performed the DFPM calculation using a multilayer model (ambient/AlAsSb alloy film/GaAs substrate). The fitting results for both real and imaginary parts of $\langle\epsilon\rangle$ are shown in Figs. 2, 3, and 4 for $x = 0.119$, 0.288, and 0.681, respectively. The fits of the DFPM (solid lines) agree well with the data (dots) for $x = 0.119$ and 0.288, with thicknesses 1835 and 1837 nm respectively. To show the quality of the fits better, we reduced the number of data points appropriately. However, we note that the fit for $x = 0.681$ cannot follow the experimental data of the sharp interference oscillation patterns below 3.5 eV, as shown in Fig. 4. In our previous study of *in situ* monitoring of the growth of AlSb on GaAs by SE, we detected imperfect growth caused by glomerulate Al before perfect laminar growth of the film [19]. Accordingly, we assumed that our $\text{AlAs}_x\text{Sb}_{1-x}$ alloy film for $x = 0.681$ has an intermediate layer on GaAs substrate and a surface-

roughness layer on the top of the film caused by the remaining effect of roughness from the agglomeration of Al. Therefore, we used a five-phase multilayer model with

FIG. 2. Pseudodielectric function spectra (dots) for $x = 0.119$ taken from Ref. [11], together with the best fit (solid lines) using DFPM.

FIG. 3. Pseudodielectric function spectra (dots) for $x = 0.288$ taken from Ref. [11], together with the best fit (solid lines) using DFPM.

FIG. 4. Pseudodielectric function spectra (dots) for $x = 0.681$ taken from Ref. [11], together with the best fit (solid lines) using DFPM.

ambient/surface roughness/AlAsSb alloy film/interface layer/GaAs substrate. The dielectric functions of the surface-roughness and interface layers were calculated using the effective-medium approximation [20] and Cauchy model, respectively. In principle, it is expected that the interface layer has absorption above its E_0 CP. However, we claim that the transparent Cauchy model is sufficient, because the probe beam cannot reach the interface layer, interrupted by the absorption of the $\text{AlAs}_x\text{Sb}_{1-x}$ alloy film above the E_0 CP.

Figure 5 shows the DFPM spectrum (solid line) obtained as a best fit to the data (open dots) for $x = 0.681$ with excellent agreement, demonstrating the validity of our analysis. The dashed lines show the contributions of the six individual CPs in Fig. 5(a). To show the quality of the fits better, we reduced the number of data points appropriately here also. The obtained thicknesses of roughness, film, and interface layers are 0.71, 1687, and 28 nm respectively. The same analysis was repeated for $x = 0.829$ yielding similar fitting quality to that seen in Fig. 5. For $x = 0.829$

the thicknesses of roughness, film, and interface layers are 0.81, 1940, and 11 nm, respectively.

To construct numerical values of ε for arbitrary compositions, we interpolated the results for all data. We represent the x dependences by the cubic equation

$$f(x) = a + bx + cx^2 + dx^3. \quad (3)$$

The best-fit parameters are given in Table 2. Figure 6 shows the As-composition dependences of E_C as an example. The open dots are parameterized values for each temperature, and the solid lines are the best fits to Eq. (3). The crossing of the E_2 and E_0' CPs is also detected in our DFPM analysis, as in a previous band-calculation study [11].

In Fig. 7 we compare the original data to the reconstruction for the representative composition $x = 0.288$. The dots and solid lines are measured and reconstructed spectra, respectively. The reconstructions are in excellent agreement with the data on this scale. Using these results we could

FIG. 5. (a) Dielectric function (open dots) for $x = 0.681$, together with the DFPM reconstruction (solid line) using six CP components (dashed lines). (b) Data (open dots) and fit (solid line) to both real and imaginary parts of $\langle \varepsilon \rangle$ in the region of oscillations.

FIG. 6. As-composition dependences of the energy parameters. The open dots are the parameters and the solid lines are fits using Eq. (3).

FIG. 7. Comparison of data (dots) to spectra (solid lines) reconstructed using the parameters of Table 2 for $x = 0.288$.

TABLE 2. Parameters for calculating the composition dependences by using Eq. (3)

	a	b	c	d
E_0 (indirect)	1.603	-0.286	0.847	0
E_0 (direct)	2.190	-0.766	1.553	0
E_1	2.851	0.221	0.841	0
$E_1+\Delta_1$	3.226	0.362	0.471	0
E_0'	3.777	0.417	0.741	0
E_2	4.114	0.150	0.432	0
E_1'	5.200	2.995	-5.765	4.071
$A(E_1)$	53.497	1223.469	-1008.687	-226.157
$A(E_1+\Delta_1)$	119.844	621.271	-76.941	-538.005
$A(E_0')$	302.243	-57.150	1232.406	-1383.811
$A(E_2)$	126.788	-142.989	911.109	-737.083
$A(E_1')$	213.087	1833.781	-2848.971	922.103
$B(E_1)$	19.061	-2.184	12.851	-15.941
$B(E_1+\Delta_1)$	20.051	-5.601	23.730	-13.148
$B(E_0')$	59.790	14.489	-50.807	-2.276
$B(E_2)$	23.874	-149.830	319.369	-137.114
$B(E_1')$	7.047	11.216	-2.660	-9.292
$A_{LM}(E_0 \text{ direct})$	0.599	-0.158	-0.382	0
$A_{LM}(E_1)$	0.084	-0.344	0.361	0
$A_{UM}(E_1+\Delta_1)$	0.367	0.785	-0.924	0
$E_{UM}(E_0')$	0.423	-0.039	0.127	-0.341
$A_{UM}(E_1')$	0.371	-1.171	1.861	-0.722

 FIG. 8. (a) Real and (b) imaginary parts of the reconstructed dielectric functions of $\text{AlAs}_x\text{Sb}_{1-x}$ for various x , as shown.

 FIG. 9. (a) Refractive index n and (b) extinction coefficient k of the reconstructed dielectric functions of $\text{AlAs}_x\text{Sb}_{1-x}$ for various x , as shown.

calculate ε for any $\text{AlAs}_x\text{Sb}_{1-x}$ alloy, as shown in Fig. 8, where panels (a) and (b) show the real and imaginary parts respectively. The spectra are offset by increments of 20 relative to that for $x = 0.1$. For convenient application in device design, we also show the complex refractive index in Fig. 9. The spectra are offset by increments of 2 relative to that for $x = 0.1$.

IV. CONCLUSION

We obtain excellent representations of the pseudo-dielectric functions of $\text{AlAs}_x\text{Sb}_{1-x}$ from 0.74 to 6.0 eV for arbitrary As composition x . Agreement is achieved with reasonable parameter values. The optical properties reported here will be useful in device design for high-speed optoelectronic applications and *in situ* monitoring of growth and deposition.

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