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Parametric modeling of the dielectric functions of $InAs_xP_{1-x}$ alloy films on InP

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ABSTRACT

We report an analytic expression that accurately represents the dielectric functions $\varepsilon = \varepsilon_1 + i\varepsilon_2$ from 1.5 to 6.0 eV of $InAs_xP_{1-x}$ alloy films over the entire composition range $0 \le x \le 1$. We use the parametric model (PM), which describes the dielectric functions of semiconductor materials as a sum of Gaussian-broadened polynomials. The dielectric function spectra are those that we obtained previously by spectroscopic ellipsometry for the specific compositions $x = 0.00$, 0.13, 0.40, 0.60, 0.80, and 1.00. The PM reconstructions are in excellent agreement with the data. With the information provided here, dielectric functions of arbitrary compositions can be calculated.

1. Introduction

InAsP ternary alloys are of interest for both infrared optoelectronic and high-speed electronic device applications due to their wide tuning range of bandgap energies from 0.35 to 1.35 eV [1–3]. In addition, the InAsP/InGaAs system potentially offers larger band offset energies compared to InGaAsP [1]. When designing devices using $InAs_xP_{1-x}$ alloys, accurate information on their optical properties is required. However, no comprehensive description of the dielectric functions $\varepsilon = \varepsilon_1 + i\varepsilon_2$ of these alloys as a function of As-composition x has been presented thus far.

In this work, we parameterize previously reported ε data of $InAs_xP_{1-x}$ alloys for compositions $x = 0.00$, 0.13, 0.40, 0.60, 0.80, and 1.00 to obtain analytic representations of ε as a function of x for $0 \le x \le 1$. This allows ε to be calculated as a continuous function of x. The original data were obtained by spectroscopic ellipsometry (SE) [4,5]. SE is an excellent technique for determining dielectric function data, since these can be obtained directly from complex reflectance ratio ρ without the need of Kramers–Kronig transformations [6–8]. To obtain analytic expressions for these data, we use the parametric model (PM) [9,10], which avoids unphysical addition of CPs to better describe experimentally obtained dielectric function. In our study we determined the parameters needed to calculate ε of $InAs_xP_{1-x}$ alloys with improved accuracy for arbitrary compositions x.

2. Modeling

We base our analysis on the <ε> spectra from 1.5 to 6.0 eV of $InAs_xP_{1-x}$ alloys that were reported previously [4,5]. In brief, a series of $InAs_xP_{1-x}$ alloys of compositions ranging from $x = 0.13$ to 0.80 was grown at ~480 °C on Fe-doped semi-insulating InP (001) substrates by chemical beam epitaxy. The <ε> spectra from 1.5 to 6.0 eV were measured by SE with the samples at room temperature. To minimize the effects of surface overlayers, all data were obtained following chemical etching. Progress was watched in real time to ensure overlayer removal to the maximum extent possible.

To obtain dielectric functions of $InAs_xP_{1-x}$ alloys for arbitrary x, we use the PM [9,10]. The PM has proven to be an accurate means of representing dielectric functions, giving excellent agreement between reconstructions and data [11–13]. In the PM the dielectric function is given as the summation of m energy-bounded Gaussian-broadened polynomials that represent critical point (CP) contributions within the accessible spectral range and P poles that represent contributions of absorption outside the interesting region to match ε_1 lineshape. The general expression is

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) = 1 + i\sum_{j=1}^{m}\int_{E_{\min}}^{E_{\max}} W_j(E)\Phi\left(\hbar\omega, E, \sigma_j\right)dE \quad (1)$$

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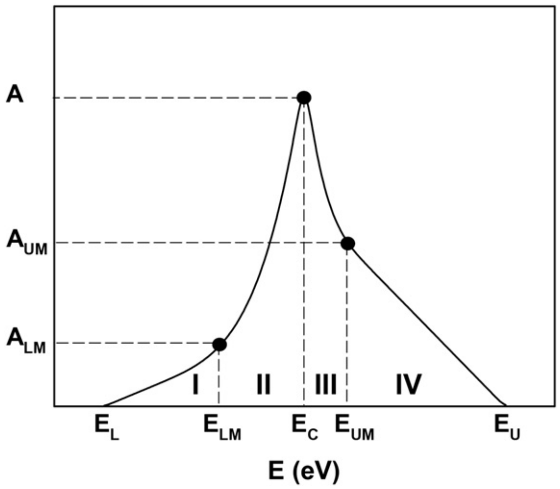

Fig. 1. A single CP structure described by the PM with four polynomial ensembles.

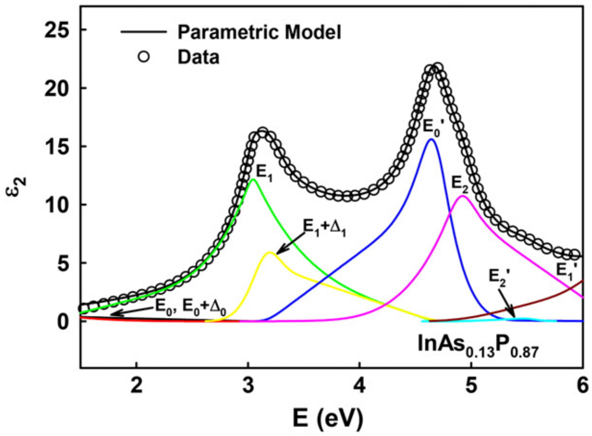

Fig. 3. Dielectric function (open dots) of $InAs_{0.13}P_{0.87}$ with the PM reconstruction (black solid line) using eight component CPs (various color solid lines). The PM describes the data with eight structures representing the E_0, $E_0 + \Delta_0$, E_1, $E_1 + \Delta_1$, E_0', E_2, E_2', and E_1' CPs.

where

$$\Phi\left(\hbar\omega, E, \sigma_j\right) = \int_0^\infty e^{i\left(\hbar\omega - E + i2\sigma^2 s\right)s} ds - \int_0^\infty e^{i\left(\hbar\omega + E + i2\sigma^2 s\right)s} ds$$
$$= \sqrt{\frac{\pi}{8\sigma^2}}\left[e^{-y_1^2} + e^{-y_1^2 erf(iy_1)} - e^{-y_2^2} - e^{-y_2^2 erf(iy_2)}\right], \tag{2a}$$

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

$$W_j(E) = \sum_{k=0}^{N} P_{j,k}{}^k E\left(uE\sigma_j\right) u\left(u_j - b\right), \tag{2c}$$

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 $(\hbar\omega + E)/\left(2\sqrt{2}\sigma\right)$ can be constructed numerically for each order of polynomial required by Eq. (2c). [9,10].

In the present work each CP is described by nine parameters, as depicted in Fig. 1. The center energies E_C correspond to the CP energy, while the bounding energies E_L and E_U delineate adjacent CPs. E_{LM} and E_{UM} are two control points for establishing the asymmetric characteristics of the lineshape. A_{LM}, A, and A_{UM} are the respective amplitudes at E_{LM}, E_C, and E_{UM}. The corresponding real part of ε is obtained by a Kramers–Kronig transformation with an extra parameter used for the baseline. To construct the lineshape of a given 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. Therefore, the PM can describe asymmetric behavior not only at the direct band gap E_0 but also at higher CPs.

3. Results and discussion

Fig. 2(a) and (b) shows the real and imaginary parts of our best ε spectra of $InAs_xP_{1-x}$ alloys obtained from Ref. 4. The spectra of InP ($x = 0.00$) and InAs ($x = 1.00$) are from previous measurements on bulk samples [5]. For clarity, ε_1 and ε_2 spectra are offset by successive increments of 10 relative to the bottom spectrum of InP, $x = 0$. The CP structures E_1, $E_1 + \Delta_1$, E_0', and E_2 can easily be observed in both ε_1 and ε_2. The identities of these features follow from previous studies [4].

Fig. 3 shows that the component CP structures combine to generate the ε_2 spectrum of $InAs_{0.13}P_{0.87}$ as an example. The open circles are data of the $InAs_{0.13}P_{0.87}$ from Fig. 2, while the solid line is the fit of the PM to these data. The dashed lines show the contributions of the component CPs. The number of data points is reduced appropriately to better

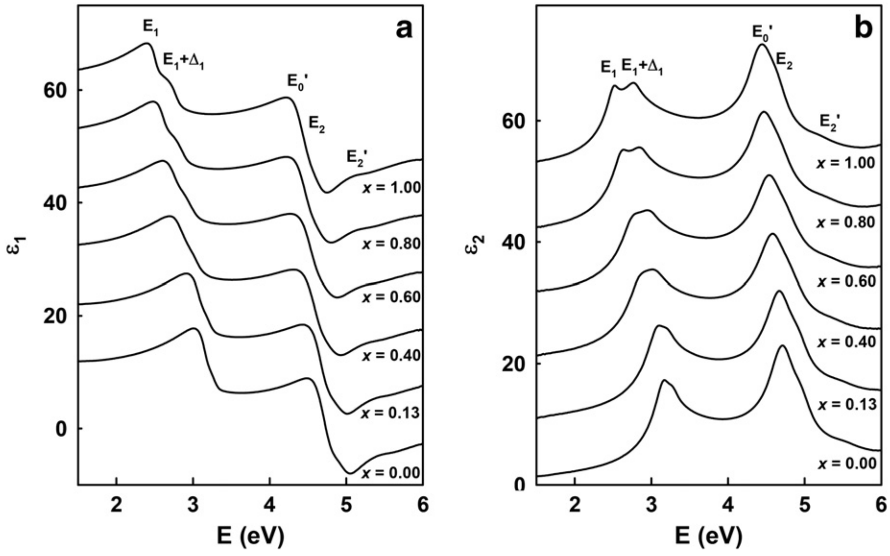

Fig. 2. (a) Real and (b) imaginary parts of the dielectric function of $InAs_xP_{1-x}$ for $x = 0.00, 0.13, 0.40, 0.60, 0.80$, and 1.00 [4,5]. The spectra are offset by 10, starting at the bottom.