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Optical properties of InP from infrared to vacuum ultraviolet studied by spectroscopic ellipsometry

Indra Subedi [a], Michael A. Slocum [b], David V. Forbes [b], Seth M. Hubbard [b], Nikolas J. Podraza [a,*]

[a] *Department of Physics & Astronomy and Wright Center for Photovoltaics Innovation & Commercialization, University of Toledo, Toledo, OH 43606, USA*
[b] *NanoPower Research Laboratory, Rochester Institute of Technology, Rochester, NY 14623, USA*

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ABSTRACT

The optical properties of an epitaxial indium phosphide (InP) film deposited on an Fe compensated InP (InP:Fe) wafer have been measured at room temperature by *ex-situ* spectroscopic ellipsometry over a spectral range of 0.038–8.5 eV. The complex dielectric function spectra, $\varepsilon\ (E) = \varepsilon_1\ (E) + i\varepsilon_2\ (E)$, have been determined by fitting a parametric model to the experimental ellipsometric data. Kramers-Kronig consistent parameterizations have been applied to describe interband transitions and defect-based sub-bandgap absorption in the 0.73–8.5 eV spectral range, and both phonon modes and free carrier properties in the 0.038–0.73 eV range. Spectra in ε from 0.73–8.5 eV shows ten higher energy interband critical point transitions at 1.36, 1.42, 3.14, 3.34, 4.71, 4.97, 5.88, 6.45, 7.88, and 8.22 eV. The direct band gap energy of 1.37 eV and Urbach energy 46 meV are also determined from spectra in ε. A strong optical phonon mode is identified near 305 cm^{-1}. Electronic transport properties, carrier concentration (N) and mobility (μ), calculated from Drude model with $N = 1.9 \times 10^{18}$ cm^{-3} and $\mu = 1559$ cm^2/Vs agree well with direct electrical Hall effect measurement values of $N = 2.2 \times 10^{18}$ cm^{-3} and $\mu = 1590$ cm^2/Vs. A parameterization of ε from 0.038 to 8.5 eV for the epitaxial InP film is reported.

1. Introduction

Indium phosphide (InP) is a III–V binary compound semiconductor made up of indium and phosphorus with a face-centered cubic zinc blende crystal structure. It has attracted significant fundamental research interest as a result of technological applications, mainly in the field of microelectronics and optoelectronics as a substrate for high-speed electrical and optoelectronic devices. The excellent lattice match that has been demonstrated between InP and a variety of other epitaxial layers has established this material as a useful substrate [1–5]. InP is also considered to be well-suited for use in vertical cavity lasers [6] and high electron mobility transistors [7]. Due to better radiation resistance than GaAs and Si, InP solar cells have been of interest for space applications [8,9]. Accurate determination of how interfaces with other materials influence InP optical properties and critical point transition energies is essential for optimizing device performances [10,11]. Variation in electrical and optical properties arising from impurities and dopant atoms such as S, Sn, Fe, and Zn have also been studied [12]. In the previous investigations into the optical response of InP [13–15], most exclude the spectral region below the first critical point, except for a study by Herzinger et al. [3] that uses spectroscopic ellipsometry to determine the pseudodielectric function for InP in the spectral range from 0.75 to 5 eV. Infrared (IR) range optical properties of InP from spectroscopic ellipsometry are not well reported at present. This work presents a room temperature *ex-situ* spectroscopic ellipsometry study of an epitaxial InP film deposited on an Fe compensated InP (InP:Fe) substrate wafer over a wide spectral range from 0.038 to 8.5 eV, spanning the IR to vacuum ultraviolet (VUV) wavelengths. These measurements are used to determine the optical response of both the InP:Fe substrate and InP epitaxial film in the form of complex dielectric function spectra, $\varepsilon\ (E) = \varepsilon_1\ (E) + i\varepsilon_2\ (E)$. Critical point (CP) interband electronic transitions at and above the band gap, an IR optical phonon mode, and electronic transport properties from the Drude model for free carrier absorption are evaluated from ε. The parametric models defining ε over each spectral range are combined to generate one model for InP from 0.038 to 8.5 eV.

* Corresponding author.
E-mail addresses: indra.subedi@rockets.utoledo.edu (I. Subedi), nikolas.podraza@utoledo.edu (N.J. Podraza).

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Table 1
Thicknesses obtained from the model fit to ellipsometric spectra collected for the epitaxial InP film on the InP:Fe wafer substrate.

Layer	Thickness from IR range analysis (0.038–0.73 eV)	Thickness from NIR – VUV range analysis (0.73–8.5 eV)
Surface Layer	9.3 ± 0.6 nm	12.2 ± 0.1 nm
InP Film	1348 ± 3 nm	1318 ± 1 nm
Substrate-Film Interface	197 ± 8 nm	365.646 ± 0.002 nm

2. Experimental details

The InP film is grown on a Veeco D125-LDM metal-organic vapor phase epitaxy (MOVPE) system at 60 Torr using trimethylindium, phosphine, and disilane sources. After baking the semi-insulating InP:Fe substrate at 580 °C for 10 min in a phosphine ambient, a nominally 1.5 μm Si doped InP layer is grown at 580 °C with a V/III ratio of 119. The orientation of the InP sample is (001) surface offcut 2° relative to the ⟨111⟩A direction. Room temperature Hall measurements are completed on a Bio-Rad HL5500 to obtain doping concentration and mobility. Epitaxial InP grown on a single crystal InP:Fe wafer is measured with two spectroscopic ellipsometers covering different spectral ranges. First, room temperature ellipsometric spectra (in $N = \cos 2\psi$, $C = \sin 2\psi \cos \Delta$, $S = \sin 2\psi \sin \Delta$) are collected at 70° angle of incidence using a near-IR extended rotating analyzer VUV variable-angle spectroscopic ellipsometer (Gen I, VU-302 VUV-VASE, J.A. Woollam Co.) [16] from 0.73 to 8.5 eV (1700–146 nm) with a spectral resolution of 0.07 nm. This VUV ellipsometer system is equipped with an automated MgF_2 Berek compensator which allows more accurate determination of the ellipsometric parameter Δ. The sample is mounted in continuous nitrogen purging environment during the measurement to minimize the effect of ambient oxygen and water vapor absorption at higher photon energies. Second, a rotating compensator Fourier transform IR ellipsometer (FTIR-VASE, J.A. Woollam Co.) [17] operating from 0.038 to 0.73 eV (32.8–1.7 μm; 304.7–5882.5 cm^{-1}) is used to acquire ellipsometric data from the same sample at 70° angle of incidence with spectral resolution of 4 cm^{-1}. Both measurements are made on the "as-deposited" sample such that it has a naturally occurring surface oxide layer and roughness.

3. Results and discussion

The structural and optical properties of the constituent layers are extracted in the form of layer thicknesses and ε, respectively, by fitting a parameterized model to measured ellipsometric spectra. Two spectral regions, 0.038–0.73 eV and 0.73–8.5 eV, are separately analyzed. Structurally, this model assumes an interfacial layer between a semi-infinite substrate and bulk epitaxial layer such that the full stack consists of the following: semi-infinite InP:Fe wafer substrate/interface/epitaxial InP film/surface layer/air ambient. Spectra in ε and layer thicknesses are determined using a least square regression analysis that minimizes an unweighted error function [18],

$$\sigma = \sqrt{\frac{1}{3n-m}\sum_{j=1}^{n}\left[\begin{array}{l}\left(\cos 2\psi_j^{\text{mod}} - \cos 2\psi_j^{\text{exp}}\right)^2\\ +\left(\sin 2\psi_j^{\text{mod}}\cos\Delta_j^{\text{mod}} - \sin 2\psi_j^{\text{exp}}\cos\Delta_j^{\text{exp}}\right)^2\\ +\left(\sin 2\psi_j^{\text{mod}}\sin\Delta_j^{\text{mod}} - \sin 2\psi_j^{\text{exp}}\sin\Delta_j^{\text{exp}}\right)^2\end{array}\right]} \quad (1)$$

where n is the number of measured values, m is the number of fit parameters, and "exp" and "mod" denote experimental and model-generated data, respectively.

In this work we are extracting ε for the InP:Fe wafer, InP epitaxial film, and the surface layer of InP. Spectra in ε for the surface layer are determined from fitting spectra from 0.73 eV to 8.5 eV using a Lorentz oscillator model [19]. For the InP film, spectra in ε from 0.73 to 8.5 eV have been analyzed as the sum of critical point parabolic band (CPPB) oscillators [20,21] at and above the lowest energy critical point (E_0) and an exponential Urbach tail below it. From 0.038–0.73 eV spectra in ε_2 for the film are represented by a Drude oscillator [22] to account for free carrier absorption and a Lorentz oscillator [19] to account for a phonon mode. For the substrate InP:Fe wafer, spectra in ε for both ranges, 0.038–0.73 eV and 0.73–8.5 eV, are modeled by a Sellmeier oscillator [19]. The thicknesses obtained from parametric modeling of all layers are summarized in Table 1. Fig. 1 compares experimental ellipsometric spectra in N, C, & S and the corresponding model fit for both IR and near-IR (NIR) – VUV data ranges.

3.1. Parametrization of InP surface layer

Analysis of spectra from 0.73 to 8.5 eV provides sensitivity to ε describing the surface layer on the outer surface of the film, which is modeled as a Lorentz oscillator model [19] and a variable constant additive term to $\varepsilon_1(\varepsilon_\infty)$ term. The expression for the Lorentz oscillator is,

$$\varepsilon(E) = \frac{A\,\Gamma E_0}{\left(E_0^2 - E^2\right) - i\,\Gamma E}, \quad (2)$$

where A is the amplitude, E_0 is the resonance energy, and Γ is the broadening. The resulting spectra in ε for this surface layer are shown in Fig. 2 and corresponding parameters are given in Table 2. After being determined through analysis of the NIR – VUV measurements, the surface layer ε is fixed for the IR range analysis, although the surface layer thickness is allowed to vary. In comparison to literature reports of ε describing InP native oxide [23], the result shown in Fig. 2 have significantly smaller amplitudes for both real and imaginary parts. Such differences from the native oxide ε could be the result of a variety of factors such as time of atmospheric exposure, varying growth conditions, or differing doping concentration of the epitaxial film. The difference in ε here may also arise from the contributions to the surface layer including the presence of surface roughness as well. Spectra in ε of the surface layer here can be described by Bruggeman effective medium approximation [24,25] of native oxide from Ref. [23] and void. Using this approach this surface layer contains a 0.406 ± 0.002 void fraction.

3.2. InP:Fe substrate and interface

A separate parameterization is used to simultaneously describe ε of the InP:Fe substrate, and consists of a single Sellmeier oscillator [19] and a ε_∞ term. The Sellmeier oscillator contributes to ε_1 only and is represented as a Lorentz oscillator with zero broadening ($\Gamma = 0$), written as

$$\varepsilon(E) = \frac{A_s}{E_s^2 - E^2}, \quad (3)$$

Table 2
Parameters describing spectra in ε for InP surface layer with $\varepsilon_\infty = 1.09 \pm 0.01$.

Oscillator	A	Γ (eV)	E_0 (eV)
Lorentz	2.63 ± 0.02	1.75 ± 0.01	8.919 ± 0.006