

THz Characterization of ITO Films on p-Si Substrates

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Abstract— This paper reports broadband THz free-space transmission measurements and modeling of indium-tin-oxide (ITO) thin films on p-doped Si substrates. Two such samples having ITO thickness of 50 and 100 nm, and DC sheet conductance 260 and 56 Ω/sq , respectively, were characterized between 0.2 and 1.2 THz using a frequency-domain spectrometer. The 50-nm-film sample displayed very flat transmittance over the 1-THz bandwidth, suggesting it is close to the critical THz sheet conductance that suppresses multi-pass interference and thereby achieves THz passive *equalization*. This is consistent with a simple transmission-line (TEM wave) model of the propagation. Also, the value of THz sheet conductance that best fits the transmittance data is roughly 50% higher than the dc value for both samples, suggesting that the ac conductivity is non-Drudian.

1. INTRODUCTION

Indium-tin oxide (ITO) has long been of interest as a transparent ohmic-contact (TOC) material for infrared detectors and other applications because of its unique optical properties and their variability by material composition [1–4]. In recent years ITO has migrated into the THz region along with interesting metamaterial-based component research also aimed at the TOC application [5–7]. Perhaps the most important study was made of ITO on semi-insulating GaAs where it was found that for a specific ITO thickness the internal reflections in a GaAs substrate can be suppressed, making the THz transmission flat with frequency [8]. A key feature of ITO in these applications is that its bulk conductivity is in the semi-metallic range, $\sigma \sim 10^4\text{--}10^5$ S/m, compared $\sigma > 10^7$ S/m for common (transition) metals, so that sheet resistances of around $\eta_o = 377 \Omega/\text{sq}$ can be obtained with film thicknesses of ~ 100 nm instead of the few-nm required of common transition metals. This makes the deposition more accurate and reproducible. However, the electrical properties of ITO depend on several material characteristics, such as the stoichiometry, and the effect of these on GHz-to-THz (RF) electrical conductivity is not yet well understood.

2. EXPERIMENTAL METHODS

For the present experiments, two ITO films having thickness 50 nm (#1) and 100 nm (#2) were deposited on p-silicon (CMOS-grade) substrates by reactive-ion-assisted, electron-beam evaporation with a stoichiometry of $\approx 10\%$ tin into indium oxide [9]. The thickness and bulk dc conductivity of the Si substrates were 393 μm and 6.0 S/m (16.7 $\Omega\text{-cm}$), respectively. The sheet resistance (conductance) of both ITO films was measured by the standard 4-point (Kelvin) dc probe technique and found to be 260 Ω/sq (3.85 mS/sq) and 56 Ω/sq (17.9 mS/sq) for films #1 and #2, respectively. Assuming uniform conduction through the films, these correspond to bulk conductivities of $\sigma_0 = 7.7 \times 10^4$ S/m for the 50-nm film, and $\sigma_0 = 1.79 \times 10^5$ S/m for the 100 nm film.

After fabrication the transmittance of a bare p-Si substrate (control sample) and the two ITO samples was measured from ≈ 200 to 1200 GHz using a diode-laser-driven photomixing spectrometer (Emcore PB7100). As described in detail previously [10], this instrument provides a combination of high resolution (~ 500 MHz), high dynamic range (~ 80 dB at 200 GHz; > 30 dB at 1.2 THz), and continuous tuning with no voids or laser mode-hops. The instrumental block diagram is shown in Figure 1 along with the location of the ITO-on-Si samples at the center point between the transmitter and receiver where the THz beam is almost perfectly collimated. For the control substrate and each of the ITO samples, three spectra are used to calculate the transmittance: (1) background spectrum $B(\nu)$ with all samples removed from the THz path, (2) noise floor $N(\nu)$ with the THz path in Figure 1 blocked by a metal plate, and (3) each of the three sample spectra $S_n(\nu)$. The individual transmittances $T_n(\nu)$ are then calculated as $T_n = [S_n(\nu) - N(\nu)]/[B(\nu) - N(\nu)]$.

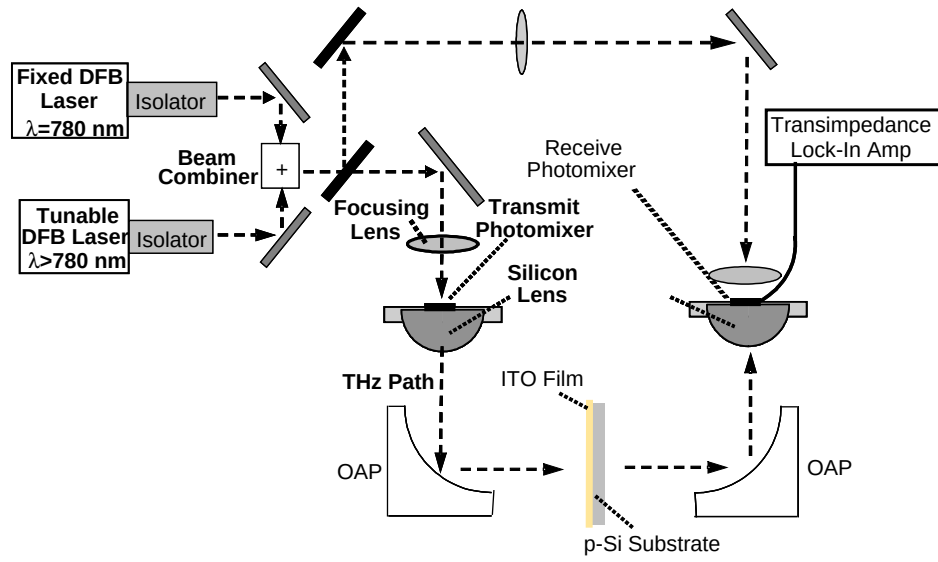


Figure 1: Instrumental block diagram for measuring ITO THz transmission vs frequency.

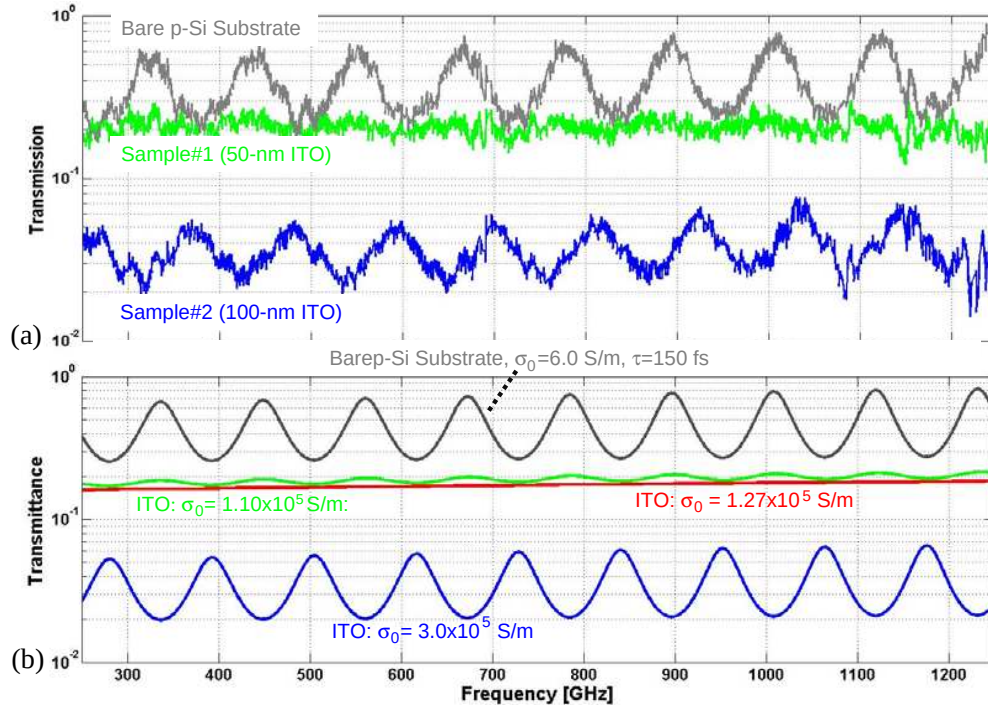


Figure 2: (a) Experimental THz transmittance for two ITO-on-Si substrates, and bare Si substrate. (b) Simulated THz transmittance for same samples as (a) plus a third ITO sample having the critical value of THz sheet conductance, which corresponds to a bulk conductivity, $\sigma = 1.27 \times 10^5$ S/m for the 50-nm-thick film. The slight upward trend in all curves is caused by the Drude-like behavior of the ac conductivity of the silicon.

3. EXPERIMENTAL RESULTS

Figure 2(a) shows the three transmittance spectra plotted on a logarithmic scale for comparative purposes. The Si control substrate shows the highest overall transmittance but also the strongest oscillation vs frequency of the three samples over the 1.0-THz bandwidth. This is caused primarily by the large real-part of dielectric function of silicon in the THz region ($\epsilon_r \approx 11.66$ [11]). The period of oscillation is very close to that expected for any lossless parallel-plate etalon, $\Delta\nu = c/(2nt) = 112$ GHz (for $n = 3.42$ and $t = 393 \mu\text{m}$). The oscillating transmittance is reminiscent of ideal dielectric-etalon optical behavior except that the low-frequency transmittance does not reach unity

at the peaks because of absorptive losses in the p-Si, presumably caused by the free holes. To better understand this we carried out numerical computations using a stratified-media, characteristic-matrix approach described in Ref. [12]. The absorptive losses in the p-Si can then be described by a complex dielectric function $\varepsilon(\omega) = \varepsilon_r \varepsilon_0 - j\sigma/\omega$ where σ is the electrical conductivity and ε_0 is the vacuum permittivity [13]. We applied the Drude model long-known to work well in crystalline semiconductors up to THz frequencies or higher at room temperature: $\sigma(\omega) = \sigma_0/(1 + j\omega\tau)$, where σ_0 is the dc bulk conductivity, τ is the momentum relaxation time, and the $+$ sign assumes a counterclockwise rotating phasor, $e^{+j\omega t}$, convention for the propagating-wave time dependence. The simulated transmittance through the bare p-Si is plotted in Figure 2(b) for $\sigma_0 = 6.0 \text{ S/m}$ consistent with dc 4-point-probe measurements, and $\tau = 150 \text{ fs}$ is determined by iteration. It mimics the experimental in all respects, especially the period of oscillation.

We then characterized the two ITO films deposited on the separate but materially-equivalent p-Si substrates, and the experimental transmittance is plotted in Figure 2(a). The transmittance of the 50-nm-thick film occurs just below the valleys of the bare-Si substrate, and the transmittance of the 100-nm film is significantly lower, as expected from the much higher dc sheet conductance of the 100-nm film ($56 \text{ } \Omega/\text{sq}$) compared to the 50-nm film ($260 \text{ } \Omega/\text{sq}$). It was surprising, however, that the 50-nm-film transmittance displayed so much less oscillation than the 100-nm transmittance. It appears that the THz transmission is “equalized” over the entire 1 THz of bandwidth — similar in effect to what has been designed into broadband telephone circuits for nearly a century [14], including modern Digital Subscriber Line (DSL) technology. So we augmented the stratified-media simulation, now including the ITO film into the model and parameterizing it by a complex THz bulk conductivity $\varepsilon(\omega) = \varepsilon_r \varepsilon_0 - j\sigma_{\text{THz}}/\omega$. We assumed that $\varepsilon_r = 1.0$ and the THz conductivity σ is a constant — a reasonable assumption given that the momentum relaxation time of electrons is probably much less than $1/\omega$ across the experimental band equal because of the ceramic nature of the ITO. The silicon-substrate parameters were the same as discussed above. By iteration once again, we determined good-fit values of $\sigma_{\text{THz}} = 1.1 \times 10^5 \text{ S/m}$ in the 50-nm film, and $\sigma_{\text{THz}} = 3.0 \times 10^5 \text{ S/m}$ in the 100-nm film. The resulting transmittance curves in Figure 2(b) are in good agreement with the corresponding experimental spectra of 2(a). Interestingly, both of these σ_{THz} values are substantially higher than the corresponding dc values measured by 4-pt probing, the 50-nm-film value being 43% higher, and the 100-nm-film value being 68% higher. This suggests that the frequency-dependent conductivity of ITO is non-Drudian.

4. PHYSICAL BASIS AND DESIGN RULE

Now we address the physical basis for the 50-nm-ITO transmittance spectrum being more *equalized* than the 100-nm spectrum, and present a useful *design rule*. The clue is the 180° phase shift in the oscillating transmittance spectrum of Figure 2 in going from the bare-Si (or 50-nm-ITO) to the 100-nm ITO. A feature of any etalon structure that can cause such a phase shift is a sign change in the reflection coefficient at one of the interfaces. From the Fresnel equations, the interfacial transmission coefficients are generally real and positive. To explore this further we display in Figure 3(a) a transmission-line-model — a simplification of the stratified-media approach — which assumes the ITO film thickness is much less than the material wavelength, and that the propagation within the Si substrate can be represented as a TEM mode on a transmission line. The model predicts a transmittance that depends on the air-ITO-Si transmission coefficient (the ratio of the transmitted to incident electric fields) and the Si-air transmission coefficient, both of which are always positive and mostly independent of frequency. However, the oscillation in the overall transmittance arises from the subsequent reflection at the Si-ITO-air interface and the (“multi-pass”) interference it creates with the first pass of radiation through the substrate.

The transmission line model predicts a Si-ITO-air reflection coefficient of

$$\Gamma = (Z_{\perp} - Z_S) / (Z_{\perp} Z_S) \quad (1)$$

where Z_S is the substrate characteristic impedance $[= \eta_0/(\varepsilon_r)^{1/2}]$, $Z_{\perp} = \eta_0 \cdot Z_{\text{ITO}}/(\eta_0 + Z_{\text{ITO}})$, Z_{ITO} is the ITO sheet impedance, and $\eta_0 = 377 \text{ } \Omega$. Clearly, Γ changes sign at the critical value $Z_{\perp} = Z_S$ where Γ is also identically zero, and therefore multi-pass interference should be suppressed. This can be re-written as $Z_S = \eta_0 \cdot Z_{\text{ITO}}/(\eta_0 + Z_{\text{ITO}})$, or solving for the critical value:

$$Z_{\text{ITO},C} = Z_S \eta_0 / (\eta_0 - Z_S). \quad (2)$$

Neglecting the imaginary part of the dielectric function of Si, we have $\varepsilon_r = 11.66$ and get $Z_S = 110.4 \text{ } \Omega/\text{sq}$. Eq. (2) then yields a value $Z_{\text{ITO}} = 156.1 \text{ } \Omega/\text{sq}$, which corresponds to a bulk conduc-

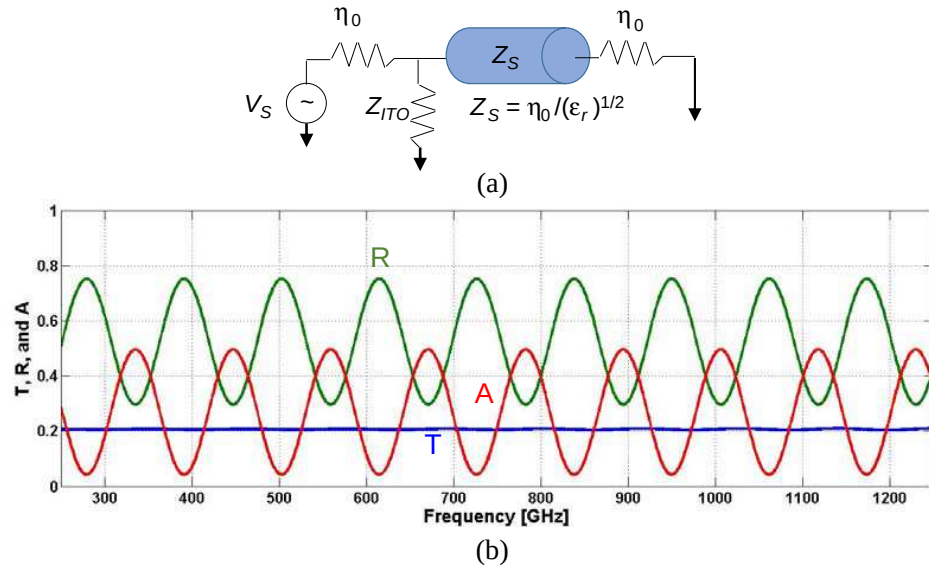


Figure 3: (a) Transmission-line equivalent circuit of the ITO-on-Si etalon. (b) Calculated values of transmittance T , reflectance R , and absorbance A for ITO film having the critical value of THz sheet conductance.

tivity of 1.28×10^5 S/m for the 50-nm-thick ITO film. Armed with this value, we repeated the stratified-medium computation for a fictitious ITO layer having these properties, and the results are shown in Figure 2(b). As predicted, the oscillations in the transmittance are almost totally suppressed, the small deviation being caused by the frequency-dependent dielectric function of Si through the Drude model. For Z_{ITO} greater than this critical value, $Z_{||}$ becomes greater than Z_S and Γ is positive according to (1). For Z_{ITO} less than this value, $Z_{||}$ is less than Z_S and Γ becomes negative.

5. DISCUSSION

Unfortunately, having the critical value of sheet impedance does not mean that standing waves are suppressed entirely, but only their effect on the forward transmittance T . To emphasize this, Figure 3(b) shows other straightforward results from the transmission-line model — the overall reflectance R and absorbance A — for the ITO-Si etalon. R is the fraction of incident power reflected back to the source, and A is the fraction absorbed, such that $T + R + A = 1$. In this case we artificially set the THz conductivity of the p-Si to zero so as not to confuse ITO absorption with Si bulk absorption. As expected, T is flat with frequency, but R and A both oscillate with the characteristic period $\Delta\nu = 112$ GHz. And they are 180° out of phase, meaning that at any frequency where the etalon displays maximum absorption, it also displays minimum reflection, and vice versa. This has implications for the use of ITO and other thin-film absorbers (e.g., graphene) in free-space-coupled THz quasi-optical components.

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