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Two-layer model for photopyroelectric spectroscopy

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ABSTRACT

This paper presents a one-dimensional theory which describes the dependence of the photopyroelectric induced signal on the optical and thermal properties of a two-layer sample, for example a thin film deposited on a substrate. Several computer simulations were performed in order to determine the validity of this model for a wide range of wavelengths and modulation frequencies.

1. INTRODUCTION

In the early 80's photopyroelectric (PPE) spectroscopy had emerged as a technique with high potentials for optical and thermal characterization of materials and devices. In 1985, Mandelis and Zver[1] developed a one-dimensional (1-D) theoretical model which covered the case of a monolayer homogeneous material. The recent developments in microelectronics especially in the field of thin films made inevitable the development of a new two-layer theory in order to make possible photopyroelectric spectroscopic measurements on thin films deposited on transparent, semitransparent, or opaque substrates. The aim of this work is to present, for the first time, a one-dimensional photopyroelectric model of a two-layer sample (film and substrate) in direct contact with an opaque pyroelectric polymer PVDF (polyvinylidene difluoride) film (black painted), and supported by a metallic backing material. Two Gaussian optical absorption coefficient spectra, $\beta_f(\lambda)$ and $\beta_s(\lambda)$, centered at different wavelengths were assumed for the film and substrate, respectively. Quantitative and qualitative predictions of the theory have been obtained by changing some experimental factors.

2. THEORETICAL MODEL

In Fig. 1, a 1-D geometry for the PPE technique in a back detection configuration is shown. Compared with the Mandelis and Zver 1-D model, an additional layer is considered: the thin film layer of thickness, L_f . This layer is irradiated with a modulated monochromatic light beam of angular frequency ω , light intensity I_{in} , and wavelength λ . The angular frequency is given by $\omega = 2\pi f_m$, where f_m is the modulation frequency. In Fig. 1, the letters g, f, s, p, and b stand for air (gas), film, substrate, pyroelectric transducer, and sample backing material respectively. The various L_j stand for the thickness of each of the above layers ($j = g, f, s, p, \text{ and } b$). The main difference of this work as compared with the one-layer model is the

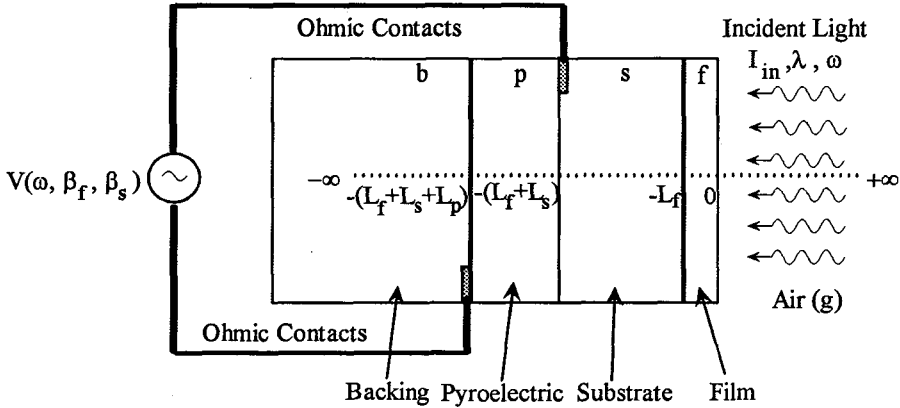


Fig. 1. One-dimensional geometry for the PPE technique in the Back Detection Configuration.

presence of an additional strong dependence of the output PPE voltage on the optical and thermal characteristics of the film, making the induced voltage a function of, ω , $\beta_f(\lambda)$, and $\beta_s(\lambda)$. This photopyroelectric voltage is given by the expression [2]:

$$V[\beta_f(\lambda), \beta_s(\lambda), \omega] = \left[\frac{pL_p\theta_p(\omega)}{K\epsilon_0} \right] \exp(i\omega t) \tag{1}$$

where p is the pyroelectric coefficient, K the dielectric constant of the pyroelectric detector and ϵ_0 is the permittivity constant of vacuum. θ_p is the average temperature across the pyroelectric film detector [3]:

$$\theta_p = \frac{1}{L_p} \left\{ \frac{1}{\sigma_p} \left[e^{-\sigma_p(L_s+L_f)} (1 - e^{-\sigma_p L_p}) C_6 + e^{\sigma_p(L_s+L_f)} (e^{\sigma_p L_p} - 1) C_7 \right] - \frac{E_p}{\beta_p} e^{-(\beta_f L_f + \beta_s L_s)} (1 - e^{-\beta_p L_p}) \right\} \tag{2}$$

where $\sigma_j \equiv (1+i)a_j$ $a_j \equiv \sqrt{\frac{\omega}{2\alpha_j}}$ (3)

3. NUMERICAL SIMULATION OF THE TWO-LAYER THEORY

The general expression of the photopyroelectric voltage, Eq.(1), combined with Eq. (2) and the analytical expressions for the constants C_6 and C_7 was evaluated numerically using a personal computer [3].

3.1. PPE Signal vs. Wavelength

For the numerical simulation of this section the following Gaussian form optical absorption coefficients were used:

$$\beta_f(\lambda) = \beta_{f0} \exp \left[- \left(\frac{4000^2}{2} \right) \left(\frac{1}{\lambda} - \frac{1}{1000} \right)^2 \right] \quad \beta_s(\lambda) = \beta_{s0} \exp \left[- \left(\frac{4000^2}{2} \right) \left(\frac{1}{\lambda} - \frac{1}{750} \right)^2 \right] \tag{4}$$

where β_{f0} and β_{s0} are well defined pre-optical absorption coefficient factors [3].

Figure 2 presents the photopyroelectric spectroscopic response (amplitude and phase) to the Gaussian absorption coefficients at two frequencies: 1 and 1000 Hz. We note that for all modulation frequencies the PPE signal decreases as the optical absorption coefficient of the film increases. In fact, the PPE amplitude

and phase have an anti-correlated behavior with respect to the optical absorption coefficient. The frequency response for three different wavelengths is presented in Fig. 3. We note that the PPE amplitude decreases as the modulation frequency increases. The PPE amplitude at 1 mHz is almost 6 orders of magnitude greater than the one at 1 kHz. In the PPE amplitude presented in Fig.3 it is easy to note the influence of the wavelength, and indirectly the influence of the absorption coefficient, on the signal amplitude. The signal amplitude is insensitive to wavelength changes for low frequencies (< 20 Hz) while at higher frequencies the amplitude decreases more quickly when the optical absorption coefficient is higher. This is due to the fact that at higher frequencies the thermal part is the only contribution that causes the PPE signal since the sample is completely opaque ($\beta_f \gg 1$).

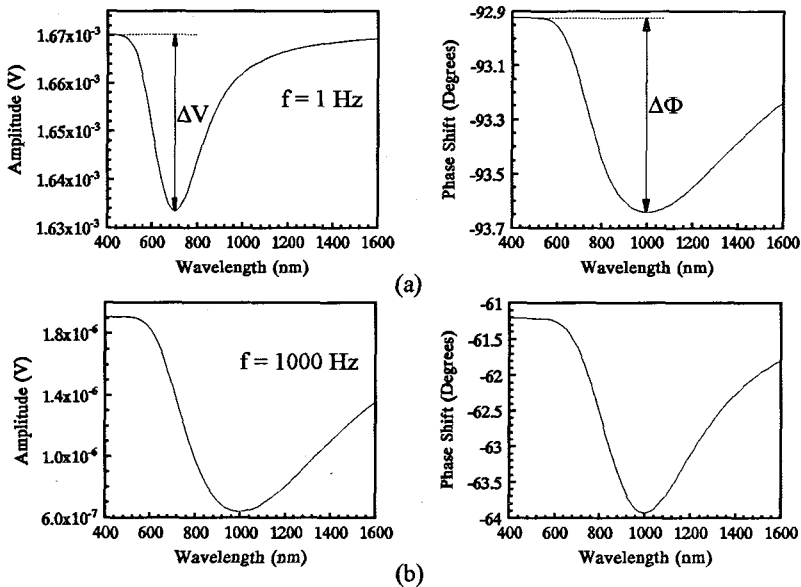


Fig. 2. PPE spectroscopic response to the Gaussian absorption coefficients for two modulation frequencies, f_m : (a) 1Hz; and (b) 1000 Hz. Film thickness, $L_f = 10 \mu m$.

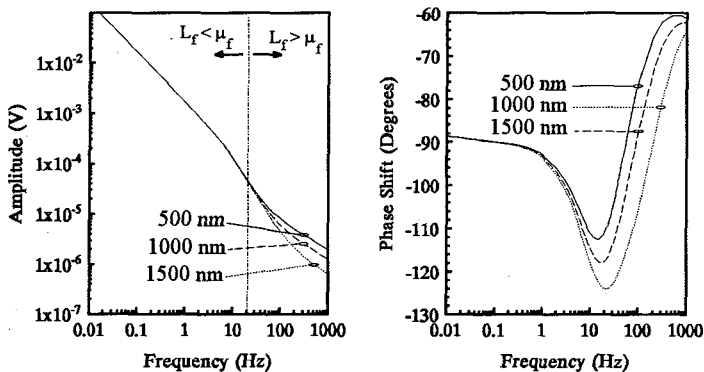


Fig. 3. PPE response as a function of the Log of the modulation frequency for three different wavelengths, λ ; 500 nm; 1000 nm; and 1500 nm. Film thickness: $L_f = 10 \mu m$.

3.2. PPE Signal vs. Frequency

Another important observation from Fig. 3 is the variation of the phase as a function of f_m . The phase shift is more sensitive to changes in the modulation frequencies as compared with changes in signal amplitude. The onset of such changes occurs between around 1 Hz. In Fig. 3 the phase decreases monotonically as a function of the modulation frequency reaching a minimum at around 20 Hz, and followed by an increase at higher frequencies. Note that the minimum phase occurs at 1000 nm where β_f is a maximum. Taking into account the thermal diffusion length of the film given by the expression, $\mu_f = \sqrt{\alpha_f / \pi f_m}$. We can evaluate the frequency limit for which we have a regime change from thermally thin condition, to thermally thick condition. This critical change occurs at the critical frequency, f_c where $L_f = \mu_f$ [4]. Substituting numerical values we calculate f_c to be 23 Hz. This is in good agreement with the slope change and phase minimum observed in Fig. 3.

3.3. PPE Signal vs. Optical Absorption Coefficient of the Thin Film

Figure 4 shows the limits of the photopyroelectric technique for the spectroscopic characterization of thin films. The data points were obtained by estimating the maximum change in the signal as a function of wavelength for different values of $\beta_f L_f$. This figure indicates that both information channels (amplitude and phase) exhibit PPE saturation at almost the same value of the product $\beta_f L_f$. We note that for $5 \times 10^{-3} \leq \beta_f L_f \leq 3$ the PPE spectroscopic technique can generate easily detectable signals.

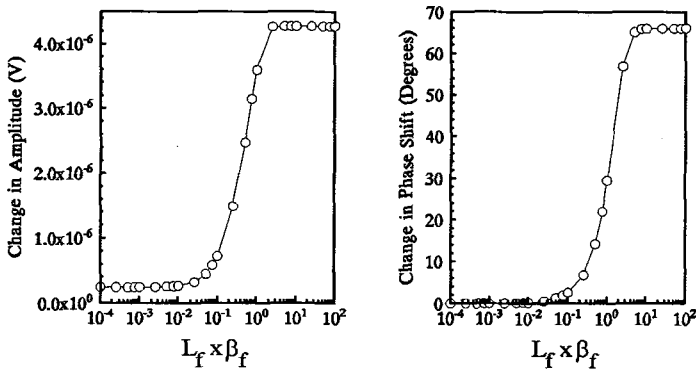


Fig. 4. PPE amplitude variation and phase shift change as a function of the product $\beta_f L_f$. ($f_m = 100$ Hz)

4. CONCLUSIONS

In this study we extended the one-layer model of Mandelis and Zver [1]. The validity of the two layer model was discussed in the light of the variation of the optical absorption coefficients of the film and substrate, as well as a function of the film thickness. Given the well known sensitivity of the PPE instrumentation and the theoretical results presented in this paper it is reasonable to say that PPE spectroscopy has an excellent future for the characterization of thin films.

5. REFERENCES

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