Mathematical reduction of the phase lag model of the photoacoustic signal to a linear dependence with the modulation frequency

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Abstract

It is presented the mathematical reduction of the phase lag model of the photoacoustic signal to a linear form for determining the thermal diffusivity in opaque solids at low modulation frequencies using the open-cell photoacoustic technique. It is shown that for $f \leq (\pi/2)^2 f_c$, where f_c is the modulation frequency at which the thermal diffusion length matches the sample thickness, the photoacoustic phase signal can be written in linear form with the modulation frequency f . Then, obtaining the proportionality coefficient by fitting the experimental data, the thermal diffusivity of the sample can be determined. The advantage of this method is that it is realized in a range of modulation frequencies below those normally used, hence, the photoacoustic signal should be alone attributed to the mechanism of thermal diffusion. Moreover, the noise-signal ratio will be less important, thus increasing the reliability of the experimental data obtained.

Keywords: Data analysis, thermal diffusivity, fotoacustic technique.

Resumen

Se presenta la reducción matemática del modelo de retardo de fase de la señal fotoacústica para la determinación de la difusividad térmica en sólidos opacos a bajas frecuencias de modulación usando la técnica fotoacústica de celda abierta. Se demuestra que para $f \leq (\pi/2)^2 f_c$, donde f_c es la frecuencia de modulación a la cual la longitud de difusión térmica iguala al espesor de la muestra, la fase de la señal fotoacústica puede escribirse en forma lineal respecto a la frecuencia de modulación f. Luego, obteniendo el coeficiente de proporcionalidad mediante el ajuste del modelo lineal a los datos experimentales, puede determinarse la difusividad térmica, a partir de dicho coeficiente y el espesor de la muestra. La ventaja de este método es que se realiza en un rango de frecuencias de modulación más bajos que los usados usualmente, por tanto, la señal fotoacústica es debida esencialmente al mecanismo de difusión de calor. Además, en este rango la razón ruido-señal decrece mejorando la confiabilidad de los datos experimentales obtenidos.

Palabras clave: Análisis de datos, difusividad térmica, técnica fotoacústica.

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I. INTRODUCTION

The open photoacoustic cell (OPC) developed for thermal characterization of solids [1], has been widely used in the measurement of the thermal properties of a large variety of materials, ranging from metals and semiconductors, to polymers and foodstuffs [2, 3, 4, 5, 6, 7]. In the OPC method the sample under study is mounted directly onto a commercial electret microphone [8] using the front chamber of the microphone as the usual gas chamber of conventional photoacoustic. Its advantage over conventional photoacoustic cells is the use of a minimal gas chamber with no further transducer medium needed, no cell machining required, and low cost. The thermal diffusivity α_s, of a sample with thickness l_s, can be determined by the OPC method by analyzing the signal amplitude or the signal phase dependence on the modulation frequency f of the incident light beam in the thermally thick regime [1, 2, 3], in which $l_s \gg \mu_s$, where $\mu_s = (\alpha_s/\pi f)^{1/2}$ is the thermal diffusion length in the sample for the frequency f. However, for materials with a high thermal diffusivity, such as metals and some semiconductors, as well as for many samples whose thickness is very small, the thermally thick regime can only be reached at modulation frequencies of hundreds or several thousands of Hz. This has two main disadvantages: i) since the PA signal decreases exponentially with the modulation frequency, the signal to noise ratio decreases quickly, resulting in lack of reliability in the analysis. Although this problem can be overcome by using a high intensity light beam this might not be appropriate because the light could be intense enough to modify the characteristics of the sample under study. ii) By increasing the modulation frequency, the thermoelastic mechanism of generation of PA signal is manifested. Since the mathematical expressions that takes into account both the heat diffusion and thermoelastic bending effect are complex, it is necessary work at higher modulation frequencies where the thermoelastic contribution is the dominant effect [1, 3].

This work report the mathematical reduction of the phase lag model of the photoacoustic signal for determining the thermal diffusivity in opaque solids at low modulation frequencies by analyzing the PA signal phase at low modulation frequencies. The predominant PA signal generating mechanism is then thermal diffusion.

II. THERMAL DIFFUSION MODEL

From the one-dimensional thermal diffusion model of Rosencwaig and Gersho [10] it is seen that the amplitude and phase difference of the OPC signal for optically opaque samples are given, respectively, by [6]

$$A = C_0 \frac{1}{f\sqrt{\cosh(2a_s l_s) - \cos(2a_s l_s)}}\ , \qquad (1)$$

$$\Delta\phi = -a\tan\left(\frac{\tan(a_s l_s)}{\tanh(a_s l_s)}\right) - \pi/2\ , \qquad (2)$$

where,

$$C_0 = \frac{\sqrt{2\alpha_s\alpha_g}V_0 I_0}{T_0 l_g k_s \pi}.$$

In these expressions α_i, l_i, k_i and a_i are the thermal diffusivity, thickness, thermal conductivity and thermal diffusion coefficient, $a_i = (\pi f\ /\alpha_i)$, of material i, respectively. Here the subscript i denotes the sample (s) and gas (g) regions. T_0 is the ambient temperature, I_0 is the incident beam intensity and V_0 is a quantity dependent on the microphone characteristics.

III. MATHEMATICAL DEVELOPMENT

Before further it is necessary to consider the following proposition:

For x in the interval $(0, (\pi/2)^2)$ it holds that,

$$A\tan\left(\frac{Tan(\sqrt{x})}{Tanh(\sqrt{x})}\right) \approx \pi/4 + x/\pi, \qquad (3)$$

with a relative error $e_{\%} < 1.2\%$, such that $e_{\%}\rightarrow$o when $x\rightarrow 0$ or when $x\rightarrow(\pi/2)^2$.

In fact, taking in account the power series representation and interval of convergence of the following basic functions:

$$Tan(x) = x + \frac{1}{3}x^3 + \frac{2}{15}x^5 + \frac{17}{315}x^7 + ...\ ;\ -\pi/2<x<\pi/2, \qquad (4)$$

$$Tan(\pi/4 + x) = 1 + 2x + 2x^2 + \frac{8}{3}x^3 + ...\ ;\ -3\pi/4<x<\pi/4, \qquad (5)$$

$$Tanh(x) = x - \frac{1}{3}x^3 + \frac{2}{15}x^5 - \frac{17}{315}x^7 + \ ...\ ;\ -\pi/2<x<\pi/2, \qquad (6)$$

and considering $y \geq 0$, it is obtained:

$$Tan(\pi/4 + y^2/\pi) = 1 + \frac{2}{\pi}y^2 + \frac{2}{\pi^2}y^4 + \frac{8}{3\pi^3}y^6 + ...\ ;\ 0\leq y<\pi/2, \qquad (7)$$

$$Tanh(y) = y - \frac{1}{3}y^3 + \frac{2}{15}y^5 - \frac{17}{315}y^7 + ...\ ;\ 0\leq y<\pi/2, \qquad (8)$$

from the theory of infinite series it holds that, the product of two convergent series also is a convergent series and its interval of convergence is the intersection of the intervals of convergence of both series. Also, the series formed by the linear combination of two converging series is converged and its interval of convergence is the intersection of the intervals of convergence of both series [11].

Therefore, the power series representation of the function $Tan(y)\cdot Tan(\pi/4+y^2/\pi)$ is convergent in the interval $[0, \pi/2)$ and is given by,

$$y + \left(\frac{2}{\pi} - \frac{1}{3}\right)y^3 + \left(\frac{2}{\pi^2} - \frac{2}{3\pi} + \frac{2}{15}\right)y^5 + \left(\frac{8}{3\pi^3} - \frac{2}{3\pi^2} + \frac{4}{15\pi} - \frac{17}{315}\right)y^7 + ...\ , \qquad (9)$$

which can be rewritten as,

$$\left(y + \frac{1}{3}y^3 + \frac{2}{15}y^5 + \frac{17}{315}y^7 + ..\right) - \left(2\left(\frac{1}{3} - \frac{1}{\pi}\right)y^3 + \frac{2}{\pi}\left(\frac{1}{3} - \frac{1}{\pi}\right)y^5 + \frac{2}{3}\left(\frac{17}{105} - \frac{2}{5\pi} + \frac{1}{\pi^2} - \frac{4}{\pi^3}\right)y^7 + ...\right), \qquad (10)$$

but, by (4) it follows that the first part of this expression is the Maclaurin series of the function $Tan(y)$, and hence,

$$Tanh(y)Tan(\pi/4 + y^2/\pi) = tan(y) - P(y)\ , \qquad (11)$$

where

$$P(y) = 2\left(\frac{1}{3} - \frac{1}{\pi}\right)y^3 + \frac{2}{\pi}\left(\frac{1}{3} - \frac{1}{\pi}\right)y^5 + \frac{2}{3}\left(\frac{17}{105} - \frac{2}{5\pi} + \frac{1}{\pi^2} - \frac{4}{\pi^3}\right)y^7 +\ ..., \qquad (12)$$

is a convergent series for all y in $[0, \pi/2)$.

From (11) it follows that,

$$Tan(\pi/4 + y^2/\pi) = \frac{Tan(y)}{Tanh(y)} - \delta(y) \quad ;\ [0, \pi/2), \qquad (13)$$

where,

$$\delta(y)=\frac{P(y)}{Tanh(y)}, \qquad (14)$$

is the error in the approximation,

$$Tan(\pi/4+y^2/\pi)\approx\frac{Tan(y)}{Tanh(y)} \quad ;[0,\ \pi/2). \qquad (15)$$

In (13) it was considered all interval [0, π/2) because for y = 0 this equation is well defined too. In fact, from (4), (6) and (12), it follows that:

$$\lim_{y\to 0}\frac{Tan(y)}{Tanh(y)}=1 \quad ;\ \lim_{y\to 0}\delta(y)=0, \qquad (16)$$

therefore, no division by zero occurs in (15) and both sides of this equality are equal to unity when $y \to 0$.

From result (16) it follows that for small values of y the error in the approximation (15) is negligible. By means of the application of the arctangent function by both sides of (15) and after realizing the change of variable:

$$y=\sqrt{x}, \qquad (17)$$

it is obtained the approximation (3), in the indicated range.

To determine an upper bound for the error in this approximation can use the graphical method since the functions involved are transcendent and continuous on this interval. The percentage relative error is given by:

$$\varepsilon_{\%}(x)=\left(\frac{a\tan\left(Tan(\sqrt{x})/Tanh(\sqrt{x})\right)}{\pi/4+x/\pi}-1\right)\times 100;\quad [0,\ (\pi/2)^2). \qquad (18)$$

In Fig. 1 is shown the graph of $\varepsilon_{\%}$ vs x. It can be observed that the error in the approximation is less than 1.2 % in all interval $[0, (\pi/2)^2)$ and that this error approaches zero when $x\to 0$ or when $x\to(\pi/2)^2$.

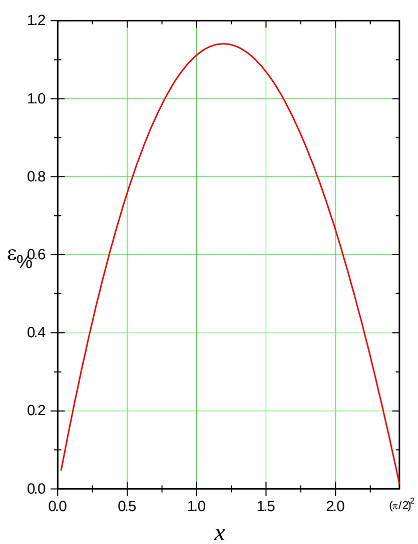

FIGURE 1. Percentage relative error of the approximation (3) given by (18).

IV. LINEAR FORM OF THE PASE LAG

Taking into account the dimensionless parameter $x = f / f_c = (a_s l_s)^2$ and the approximation (3), the phase lag of the photoacoustic signal, given by (2), can be reduced to next linear dependence with f,

$$\Delta\phi\approx-\frac{1}{\pi f_c}f-3\pi/4, \qquad (19)$$

which is valid in the interval $f \leq (\pi/2)^2 f_c$. Here, the characteristic frequency $f_c = \alpha_s/\pi l_s^2$, represents the modulation frequency at which the thermal diffusion length $\mu_s = a_s^{-1}$ matches the sample thickness. Figure 2 show the graph of $\Delta\varphi$ vs x for Eq. (2), black line, and for Eq. (19), red line.

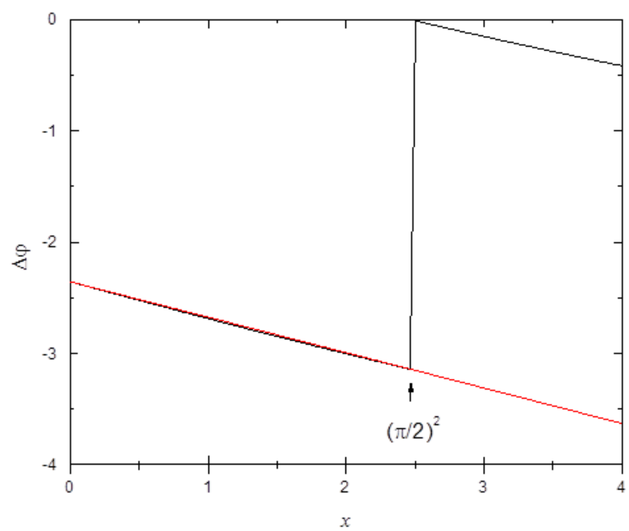

FIGURE 2. Phase lag vs $x = f / f_c$. Eq. (2) is represented by the black line and Eq. (19) by the red line.

From Fig. 2 it follows that Eq. (19) agree very well with Eq. (2) in the interval $0 < x \leq (\pi/2)^2$, hence, the linear form given for the phase lag in Eq. (19) can be used to replace Eq. (2) for frequencies less than $(\pi/2)^2 f_c$.

From Eq. (19) it can be observed that the phase lag decreases linearly with the modulation frequency in the range $f \leq (\pi/2)^2 f_c$ with a slope equal to $-1/\pi f_c$. Hence, by fitting Eq. (19) to the experimental photoacoustic phase signal can be obtained easily the characteristic frequency $f_c = \alpha_s/\pi l_s^2$. Then, the thermal diffusivity α_s of the sample is obtained when is know the thickness of the sample l_s [6].

The utility of Eq. (19) in determining the thermal diffusivity of a material from the experimental data of the photoacoustic signal has been widely reported since its introduction [6, 12, 13, 14, 15], however, is in this work where the mathematical development that reduces equation (2) to the linear form given by (19) is reported now for the first time.

V. CONCLUSIONS

It is presented the mathematical reduction of the phase lag model of the photoacoustic signal to a linear form for determining the thermal diffusivity in opaque solids at low modulation frequencies using the open-cell photoacoustic technique. It is shown that for $f \leq (\pi/2)^2 f_c$, where f_c is the modulation frequency at which the thermal diffusion length matches the sample thickness, the photoacoustic phase signal can be written in linear form with the modulation frequency f . Then, obtaining the proportionality coefficient by fitting the experimental data, the thermal diffusivity of the sample can be determined. The advantage of this method is that it is realized in a range of modulation frequencies below those normally used, hence, the photoacoustic signal should be alone attributed to the mechanism of thermal diffusion. Moreover, the noise-signal ratio will be less important, thus increasing the reliability of the experimental data obtained.

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