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Photothermal frequency-domain depth profilometry of a discrete inhomogeneous surface layer on homogeneous substrate

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Abstract

A technique for obtaining thermal diffusivity depth profiles of inhomogeneities in two-layered systems is discussed. The method uses incremental differences in the photothermal signal frequency response of a sample with the inhomogeneous surface layer compared to a homogeneous reference sample. Applications to machined steel samples are reported.

1. INTRODUCTION

In recently published work, a continuum approach to the photothermal depth profilometric problem of inhomogeneous, semi-infinite condensed phases was found to be successful in reconstructing depth-dependent thermal diffusivity profiles, using photoacoustic gas-cell [1] or infrared photothermal radiometric (PTR) [2] detection. The main feature of those approaches was the measurement of the thermal-wave frequency response (amplitude and phase) of a continuously inhomogeneous solid sample, normalized by the response of a semi-infinite homogeneous reference sample.

In this work, the earlier formulation is extended to the technologically important case of a two-layered solid consisting of a semi-infinite, homogeneous substrate supporting an inhomogeneous surface layer of thickness L . Such configurations arise, for example, in plasma spraying/coating of metals.

2. THEORETICAL

Figure 1 shows the assumed (ideal) geometry. The a.c. temperature profile in each region: air (g); investigated layer (IL or s); and substrate (b) is generated by a modulated laser beam with sufficient lateral extent so as to create a one-dimensional thermal-wave profile in the structure of Fig.1. The intensity of the beam is modulated at an angular frequency ω . The a.c. temperature fields are:

$$\begin{aligned}
 \text{(a) Gas:} \quad T_g(x, \omega) &= \Theta \cdot e^{\sigma_g x} & ; x \leq 0 \\
 \text{(b) Solid:} \quad T_s(x, \omega) &= T_s(0) \cdot \sqrt{R(x)} [C_1 e^{iH(x)} - C_2 e^{-iH(x)}] & ; 0 \leq x \leq L \\
 \text{(c) Bulk substrate; } T_b(x, \omega) &= U \cdot e^{-\sigma_b(x-L)} & ; x \geq L
 \end{aligned} \tag{1}$$

Figure 1. One-dimensional geometry of a discrete inhomogeneous surface layer on a homogeneous semi-infinite substrate.

Eqs.(1a), (1c) are standard solutions to the thermal-wave equation in homogeneous semi-infinite media [3]. Eq.(1b) is the result of a treatment of the inhomogeneous layer thermal-wave field in terms of the Hamilton-Jacobi formulation of the problem [4]. In Eqs. (1) the following definitions were made:

$\omega = 2\pi f$: angular modulation frequency of the optical intensity

$\sigma_j(\omega) \equiv (1+i) \sqrt{\frac{\omega}{2\alpha_j}}$; α_j : diffusivity of the j-th (homogeneous) medium (j:g,b)

$R(x) \equiv \frac{e_s(0)}{e_s(x)}$; $e_s(y)$: thermal effusivity of the IL at $x=y$

L : thickness of the inhomogeneous layer

$H(x) \equiv \int_0^x \sigma_s(y, \omega) dy$: σ_s is defined analogously to σ_j ; $\sigma_s(y, \omega) = (1+i) \sqrt{\frac{\omega}{2\alpha_s(y)}}$

where $\alpha_s(y)$ is the thermal diffusivity of the IL at $x=y$. C_p , C_s , Θ , $T_s(0)$ and U are constants of integration to be determined by boundary and limiting conditions. The IL is assumed to be strictly opaque, i.e. its optical penetration depth is much shorter than the shortest thermal diffusion length, $\mu_s(\omega) = (2\alpha_s/\omega)^{1/2}$, in this layer. At the interface $x=L$, continuity of temperature and heat flux (standard treatment) is assumed. To proceed further, an expression for the (assumed arbitrary) $\alpha_s(x)$ profile must be used, in order to obtain explicit expressions for $H(x)$. A simulated function which is convenient in simplifying the integration involved is [4,5]

$$\alpha_s(x) = \alpha_0 \left(\frac{1 + \Delta e^{-qx}}{1 + \Delta} \right)^2 \quad (2)$$

such that $\alpha_s(L) = \alpha_L$, $\alpha_s(0) = \alpha_0$ and

$$\Delta = \frac{1 - \sqrt{\alpha_L/\alpha_0}}{\sqrt{\alpha_L/\alpha_0} - e^{-qL}} \quad (3)$$

The parameter q is a constant to be determined from experimental data of photothermal signals (amplitude and phase) vs. frequency ω . Insertion of Eqs. (2) and (3) in the integral for $H(L)$ yields:

$$H(L) = (1+i) \sqrt{\frac{\omega}{2\alpha_L}} \left[\frac{1 - e^{-qL}}{1 - \sqrt{(\alpha_0/\alpha_L)} e^{-qL}} \right] \left[L - \frac{1}{2q} \ln \left(\frac{\alpha_0}{\alpha_L} \right) \right] \quad (4)$$

Finally, writing out the resulting thermal-wave field for a non-homogeneous IL gives:

$$T_s(0) = \frac{Q_0}{k_s(0)\sigma_s(0)} \left[\frac{1 + \gamma_{bs} e^{-2H(L)}}{1 - \gamma_{bs} e^{-2H(L)}} \left(1 + G_L(\omega) \left[\frac{1 + \gamma_{bs} e^{-2H(L)}}{1 - \gamma_{bs} e^{-2H(L)}} \right] \right) \right] \quad (5)$$

where

$$G_L(\omega) = \frac{1}{4} \sqrt{R(L)} \exp \left[- \frac{(1+i)\sqrt{\omega}}{2\sqrt{2}q} \cdot \frac{1}{\sqrt{\alpha_L}} \ln \left(\frac{\alpha_0}{\alpha_L} \right) \right] \quad (6)$$

The coupling coefficient γ_{bs} at the back interface is given by

$$\gamma = \frac{1 - b_{bs}}{1 + b_{bs}} \text{ where } b_{bs} = \frac{\sigma_b k_b}{\sigma_s(L) k_s(L)} = \frac{k_b \sqrt{\alpha_s(L)}}{k_s(L) \sqrt{\alpha_b}}.$$

3. COMPUTATIONAL AND NUMERICAL CONSIDERATIONS OF THE INVERSE PROBLEM ALGORITHM

The surface temperature response to the incident light beam on the investigated system (sample) is normalized by the surface temperature response to the same beam of the same frequency on a semi-infinite homogeneous material (reference). This gives for each frequency a data-pair: amplitude ratio and phase difference between sample and reference. The normalizing procedure is necessary for the correct accounting of all frequency dependencies in the experimental system, other than that due to the IL (ie. the instrumental transfer function). Theoretical values of the data-pair are calculated by Eq.(5):

$$|M(\omega)| \cdot e^{i\Delta\phi(\omega)} = \frac{k_{ref}\sigma_{ref}}{k_s(0)\sigma_s(0)} \cdot \left[\frac{1 + \gamma_{bs}(L) e^{-2H(L)}}{1 - \gamma_{bs}(L) e^{-2H(L)}} \left(1 + G(\omega) \left[\frac{1 + \gamma_{bs}(L) e^{-2H(L)}}{1 - \gamma_{bs}(L) e^{-2H(L)}} \right] \right) \right] \quad (7)$$

$|M(\omega)|$ is the amplitude ratio and $\Delta\phi(\omega)$ is the phase difference at angular frequency ω . To be able to calculate thermal diffusivity $\alpha_s(x)_{(j)}$ and depth $x_{(j)}$ corresponding to frequency $\omega_{(j)}$, one has to find the unknown parameters $\alpha_{0(j)}$ and $q_{(j)}$. For this task the two-dimensional Broyden's method [4] was used. The procedures had to be customized for Eq.(7) to avoid run time errors and singularities in Broyden's two-dimensional line search procedure. The method looks for $\alpha_{0(j)}$ and q_j to satisfy the minimum condition $|M_{exp}(\omega_j)| - |M_{theor}(\omega_j)| = 0$ and $\Delta\phi_{exp}(\omega_j) - \Delta\phi_{theor}(\omega_j) = 0$ for each angular frequency ω_j . Search start from the lowest frequency ω_1 .

In the following examples we tested the fidelity of the foregoing method for the reconstruction of known thermal diffusivity depth-profiles. Figure 2 shows four simulated profiles and the corresponding reconstructions in a geometry consisting of a thin solid layer on an arbitrary homogeneous semi-infinite substrate. The reconstructions are in excellent agreement with the original profiles.

Figure 2. Simulated (solid lines) and reconstructed (triangles and squares) profiles of two homogeneous (1,2) and two inhomogeneous (3,4) samples.

Figure 3. Reconstructed profile from a machined steel plate of thickness $L=250\mu\text{m}$.

4. EXPERIMENTAL

The semi-infinite approximation to the foregoing algorithm was then used to obtain the thermal diffusivity profiles of machined low carbon stainless steel plates of different thicknesses using PTR detection [2]. Air was used as bulk substrate which allowed probing, thermal diffusivity reconstruction and depth-profile generation from both sides of the sample. Figure 3 shows the reconstructed profile for the $250\mu\text{m}$ thick sample. The machining process appears to disturb the thermophysical properties of low-carbon steel down to depth of *ca.* $30\mu\text{m}$, while the material bulk remains undisturbed at *approx.* $4.8 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ in good agreement with literature values.

In conclusion, the present method can successfully reconstruct diffusivity profiles of discrete inhomogeneous layers on homogeneous substrates. In particular stainless steel thermal diffusivity profiles due to machining process were obtained clearly showing the near-surface depth range of machining damage for the first time. Further investigations are now possible on the effect of machining on material properties (thermophysical and mechanical), possibly leading to a better manufacturing control of the process.

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