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Modelling of the thermo-elastic response of composite media by a transfer matrix approach

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Abstract: A transfer matrix method is introduced here and it is demonstrated to be generally applicable for the calculation of the thermo-elastic response of one dimensional structures exposed to transient laser heating. The method enables the modelling of photothermal measurements of many practically important samples such as multi-layers and materials with continuously varying thermal and/or elastic properties. Examples for its possible applications are given.

1. THE TRANSFER MATRIX FORMALISM

Modelling the thermo-elastic response of a sample subjected to time varying photon-induced heating requires the solution of the following equations:

$$K \frac{\partial T(x,t)}{\partial x} + j(x,t) = 0, \quad (1a)$$

$$\rho c_v \frac{\partial T(x,t)}{\partial t} + \frac{\partial j(x,t)}{\partial x} = \beta H(x,t), \quad (1b)$$

$$\frac{\partial \sigma(x,t)}{\partial x} - \rho \frac{\partial^2 u(x,t)}{\partial t^2} = 0, \quad (1c)$$

$$\sigma(x,t) = c \frac{\partial u(x,t)}{\partial x} - \lambda T(x,t), \quad (1d)$$

where $T(x,t)$, $j(x,t)$, $H(x,t)$, $u(x,t)$ and $\sigma(x,t)$ denote the temperature, the heat flux, the radiation intensity, the elastic-displacement and the elastic stress, respectively. The material parameters: the optical absorption coefficient (β), the thermal conductivity (K), the density (ρ), the heat capacity (c_v), the (1111) element of the elastic-stiffness tensor (c) and the (11) element of the temperature-stress tensor (λ) are also used. Assuming that the radiation intensity follows the so called Beer's law one can write

$$H(x) = H_0 e^{-\beta(x-x_0)}, \quad (2)$$

with H_0 being the radiation intensity at a reference plane x_0 . The experimental conditions under which these one dimensional equations are valid have been discussed elsewhere[1]. To solve these equations for a sample consisting of N homogeneous layers, one can start by solving the above equations for a

(1) On leave of absences from the Institute of Isotopes of the Hungarian Academy of Sciences

homogeneous layer. This can be done by using the method of Laplace transforms [2]. The solution can be written as

$$T(x,s) = Ae^{-\mu x} + Be^{\mu x} + K_1 H(x,s), \quad (3a)$$

$$j(x,s) = \frac{1}{Z} (Ae^{-\mu x} - Be^{\mu x}) + K_2 H(x,s), \quad (3b)$$

$$u(x,s) = Ce^{-kx} + De^{kx} + G_1 j(x,s) + G_2 H(x,s), \quad (3c)$$

$$\sigma(x,s) = \frac{1}{R} (Ce^{-kx} - De^{kx}) + G_3 T(x,s) + G_4 H(x,s). \quad (3d)$$

s is the Laplace variable, A, B, C and D are free parameters determined by the boundary conditions. Other parameters are

$$\mu^2 = \frac{s\rho c_v}{K}, \quad k^2 = \frac{s\rho}{c}, \quad Z = \frac{1}{K\mu}, \quad R = -\frac{1}{ck},$$

$$K_1 = \frac{\beta}{s\rho c_v - \beta^2 K}, \quad K_2 = \frac{\beta^2 K}{s\rho c_v - \beta^2 K},$$

$$G_1 = \frac{\mu\lambda Z}{s^2\rho - c\mu^2}, \quad G_2 = \frac{\lambda\beta K_1}{s^2\rho - c\beta^2} - \frac{\mu\lambda Z K_2}{s^2\rho - c\mu^2},$$

$$G_3 = -s^2\rho K G_1, \quad G_4 = -\frac{s^2\rho}{\beta} G_2.$$

In the transfer matrix formalism the relationship for the thermo-elastic variables at the boundaries $x = x_{i-1}$ and $x = x_i$ of the i^{th} layer having the thickness $L = x_i - x_{i-1}$ ($x_i > x_{i-1}$) can be written as

$$\bar{\alpha}_i(x_i, s) = \bar{A}_i \bar{\alpha}_{i-1}(x_{i-1}, s), \quad (4)$$

where α_{i-1} and α_i refers to the vector

$$\bar{\alpha}(x, s) = \begin{bmatrix} H(x, s) \\ T(x, s) \\ j(x, s) \\ u(x, s) \\ \sigma(x, s) \end{bmatrix} \quad (5)$$

at $x = x_{i-1}$ and $x = x_i$ respectively. The transfer matrix can be written in the form

$$\bar{A} = \begin{bmatrix} e^{-\beta L} & 0 & 0 & 0 & 0 \\ A_{21} & ch(\mu L) & -Zsh(\mu L) & 0 & 0 \\ A_{31} & -\frac{sh(\mu L)}{Z} & ch(\mu L) & 0 & 0 \\ A_{41} & RG_3sh(kL) - \frac{G_1}{Z}sh(\mu L) & G_1[ch(\mu L) - ch(kL)] & ch(\mu L) & -Rsh(\mu L) \\ A_{51} & G_3[ch(\mu L) - ch(kL)] & \frac{G_1}{R}sh(kL) - G_3Zsh(\mu L) & -\frac{sh(\mu L)}{R} & ch(\mu L) \end{bmatrix} \quad (6)$$

For the sake of simplicity, the subscript i was omitted in the above equation and the following abbreviations were introduced:

$$A_{21} = K_1[e^{-\beta L} - ch(\mu L)] + ZK_2 sh(\mu L) ,$$

$$A_{31} = K_2[e^{-\beta L} - ch(\mu L)] + \frac{K_1}{Z} sh(\mu L) ,$$

$$A_{41} = G_1 K_2[e^{-\beta L} - ch(\mu L)] + G_2[e^{-\beta L} - ch(kL)] + \frac{G_1 K_1}{Z} sh(\mu L) + RG_4 sh(kL) ,$$

$$A_{51} = G_3 K_1[e^{-\beta L} - ch(kL)] + G_4[e^{-\beta L} - ch(kL)] + ZG_3 K_2 sh(\mu L) + \frac{G_2}{R} sh(kL) .$$

The advantage of using the transfer matrix concept is that the transfer matrix of a sample consisting of N layers is simply the product of those of the individual layers i.e.:

$$\bar{\alpha}_{rear} = (\bar{A}_N \dots \bar{A}_1) \bar{\alpha}_{front} , \quad (7)$$

where α_{rear} and α_{front} are α at the rear and front side of the sample, respectively.

Imposing appropriate boundary conditions at the rear and the front side of the samples makes the solution in the Laplace space complete. To get the time dependence of the thermo-elastic variable one has to specify the time dependence of the source term, and its Laplace transform. In many cases the light intensity can be approximated with the form of a Hanning function:

$$H(t) = H_0 \sin^2\left(\frac{\pi t}{\tau}\right) \quad 0 \leq t \leq \tau \quad (8a)$$

$$H(t) = 0 \quad t < 0 \text{ and } t > \tau , \quad (8b)$$

The corresponding Laplace transform is

$$H(s) = 2\pi^2 H_0 \frac{1 - e^{-\tau s}}{s[4\pi^2 + (\tau s)^2]} . \quad (8c)$$

The inverse Laplace transformation may be accomplished by numerical methods.

2. EXAMPLES

2.1 The photopyroelectric detection scheme

As an application of the transfer matrix method consider the so called photopyroelectric detection scheme[3,4], where the temperature change in the sample induces a charge (Q) on a pyroelectric material confined between $x = x_{i-1}$ and $x = x_i$

$$Q \propto \int_{x_{i-1}}^{x_i} T(x) dx \quad (9)$$

Let this detector constitute the i^{th} layer of the sample (other layers might for example be those of the sample, the fluid in connection with the sample and the backing material on which the detector is placed). Following the modelling steps described above, the temperature and the heat flux at one side of the detector may easily be calculated. (For example T_{i-1} and j_{i-1} at $x = x_{i-1}$) Then the detector signal (S) can be expressed as

$$S \propto p \left[\frac{sh(\mu L)}{\mu} T_{i-1} - \frac{Z}{\mu} [ch(\mu L) - 1] j_{i-1} - \left\{ \frac{K_2 Z}{\mu} [ch(\mu L) + 1] + \frac{K_1}{\mu} sh(\mu L) + \frac{K_1}{\beta} [e^{-\beta L} - 1] \right\} H_{i-1} \right] \quad (10)$$

A similar but more complicated expression can be also deduced for the photo-piezoelectric signal.

2.2 Continuously varying thermal conductivity profiles

Continuously varying profiles can be well approximated by many homogeneous layers if the number of the layers is large enough. As an example the following thermal conductivity profile [5] was considered:

$$K(x) = K_0 - K_1 \exp \left[-\frac{|x-A|}{B} \right], \quad (11)$$

with the material parameters those of silicon [2], $K_0 = 148 \text{ W/m/K}$, $K_1 = K_0/3$, with different values of a and b . A transient heating of such a sample with a laser pulse duration $\tau = 5 \text{ ps}$ has been modelled. In Fig. 1. surface temperature changes in percentage relative to the homogeneous sample ($K_1 = 0$) are plotted as a function of time. The dependence of the traces on parameters A and B clearly shows the possibility of depth-profiling of material with continuous thermal profiles such as generated by ion implantation.

Figure 1. Normalised surface temperature vs. time for samples with thermal conductivity variation as given in Eq. 11. Curve a: $A = 100 \text{ nm}$, $B = 20 \text{ nm}$; curve b: $A = 100 \text{ nm}$, $B = 40 \text{ nm}$; curve c: $A = 50 \text{ nm}$, $B = 20 \text{ nm}$

2.3 Multi-layered thin films

The possibility of time resolved thermal transport measurements in compositionally modulated films and the characterisation of the interfaces with picosecond transient reflectance methods has been demonstrated [6]. The transfer matrix introduced here may be an efficient calculation method for modelling such experiments. Let us recall, however, that modelling picosecond transient reflectance measurements on metals always requires the distributed nature of the light reflection to be taken into account [1], otherwise the deduced thermal parameters may be subjected to large errors.

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