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Thermal waves in materials with inhomogeneous thermal conductivity

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Abstract: Plane thermal waves in media with linearly varying thermal conductivity are analyzed, where we allow for an internal heat source arising from optical absorption. Then we apply the result to calculate the surface temperature of a semi-infinite solid in a photothermal experiment. We show how we can infer an inverse procedure that is able to yield, from only a few experimental data, a linear conductivity profile that reveals the most important aspects of the actual profile.

1. INTRODUCTION

Thermal waves in materials with homogeneous thermal parameters have been well-understood for a long time and have become standard textbook material. In layered materials, i.e. materials in which the thermal parameters vary in a stepwise manner along a single direction, exact forward calculation remains possible [1,2].

There are lots of situations, however, where material parameters vary continuously rather than discontinuously within the material, especially in the vicinity of the surface. This is, for example, the case in surface-hardened steel, where the conductivity profile reflects the hardening profile. Unfortunately, thermal wave behavior in such situations is much less well-understood since no general exact analytic solution of the problem exists. This is no real obstacle in the forward problem, since then one can look at the material as consisting of very many very thin layers. However, the large number of layers is prohibitive for the more interesting inverse problem, the calculation of the material properties from experimental data on the wave behavior. Various continuous approaches of the problem have been made, and an overview can be found in refs. [3,4].

In some of the most interesting cases, as that mentioned before, only the thermal conductivity appreciably changes as a function of the depth under the surface, whereas the density and specific heat are more or less constant. For the case of a thermal conductivity that varies linearly in the surface layer, we have presented in ref.[5] exact equations for the photothermal response in a semi-infinite solid heated by modulated incident light. A linear thermal conductivity can be viewed as a first order approximation to a variable conductivity. Especially in an inverse determination the approach is valuable, since there are only a few parameters to be determined. In earlier work [5] we have shown that we can easily extract from the surface temperature in a photothermal setup a linear conductivity profile that reveals important aspects of the actual profile. Here we present an alternative inversion procedure and will compare it with our approach of ref.[5].

2. THEORY AND RESULTS

In a photothermal experiment [6] the perpendicular incidence of laser light with periodically modulated intensity

$$I = I_0(1 + e^{i\omega t}) / 2 \quad (1)$$

on a material with thermal conductivity κ given by

$$\kappa(x) = \kappa_0 + \kappa' x, \quad (2)$$

gives rise to a time dependent temperature response, which can be written as

$$T(x, t) = \theta(x) e^{i\omega t}. \quad (3)$$

If we now introduce the new variable

$$y = 2 \frac{\sqrt{A \kappa(x)}}{\kappa'}, \quad (4)$$

$$A = -i\omega\rho c, \quad (5)$$

ref.[5] arrived at the rigorous result

$$\theta(x) = C_1 J_0(y) + C_2 N_0(y) + r\pi \left(-J_0(y) \int_{u_0}^u e^{-\gamma w} N_0(2\sqrt{w}) dw + N_0(y) \int_{u_0}^u e^{-\gamma w} J_0(2\sqrt{w}) dw \right) \quad (6)$$

where

$$u = y^2 / 4 \quad (u_0 = u(x=0)), \quad (7)$$

$$\gamma = \frac{\beta \kappa'}{A}, \quad (8)$$

$$r = -\frac{\beta I_0}{2A} e^{\beta \kappa_0 / \kappa'}, \quad (9)$$

β is the optical absorption coefficient and J_0 and N_0 denote the zeroth order Bessel and Neumann functions. In a semi-infinite solid, the conductivity cannot keep on changing with depth, for then it would be boundless. Therefore we assumed that it varies in a linear way from a value κ_0 at the surface to the value κ_1 at some characteristic depth d , and is constant beyond it. As Fig. 6a of ref.[7] suggests, this kind of profile can very well approximate a real profile.

In an experiment one measures the surface temperature θ_0 . Here we restrict ourselves to an optically opaque solid. In that case we have shown that energy conservation and continuity of temperature lead to the result

$$\theta_0 = \frac{I_0}{2} \frac{1}{i\kappa \sigma_0} \frac{N_{00}(J_{01} - iJ_{11}) - J_{00}(N_{01} - iN_{11})}{N_{10}(J_{01} - iJ_{11}) - J_{10}(N_{01} - iN_{11})}. \quad (10)$$

with

$$\sigma_j = \frac{1+i}{\sqrt{2}} \sqrt{\frac{\omega \rho c}{\kappa_j}} \quad (11)$$

$$J_{kl} = J_k(y_l) \quad ; \quad N_{kl} = N_k(y_l) \quad , \quad (12)$$

and subscript 0 or 1 means evaluation at the surface or at depth d.

It is interesting to consider the ratio of this to the result for a solid with a constant conductivity equal to the bulk value. We found [5]

$$R = \frac{\theta_0}{\theta_{0b}} = \frac{\sqrt{\kappa_1}}{\sqrt{\kappa_0}} \frac{N_{00}(J_{01} - iJ_{11}) - J_{00}(N_{01} - iN_{11})}{iN_{10}(J_{01} - iJ_{11}) - iJ_{10}(N_{01} - iN_{11})} \quad (13)$$

which e.g. can represent the relative signals of surface-hardened to unhardened material. The use of R has the advantage that it should be equal to the ratio of the measured signals, which themselves are only proportional to the surface temperature.

The key point now is that we will invert eq.(13) to find a linear profile, and hope for good resemblance with the actual profile. In principle we should try to obtain a representative value for κ_0 , κ_1 and d. However, one can easily verify that $R(\omega)$ is invariant under a simultaneous transformation $\kappa \rightarrow a^2 \kappa$ and $d \rightarrow ad$. This means that one of the parameters should be known in advance. Quite often, either the bulk value or surface value of the conductivity will be known. $R(\omega)$ is also invariant under the simultaneous transformation $\omega \rightarrow \omega/a^2$ and $d \rightarrow ad$, and we will take advantage of this. It means that d only influences the frequency scale, and not the aspect of $|R(\omega)|$.

The determination of the parameters can proceed as follows. Suppose we already know κ_1 . A direct inversion of eq.(13) based on two frequency data is not obvious, since it takes the solution of a set of two rather complicated implicit equations which could be ill-conditioned. The asymptotic expansion of the amplitude of eq.(13) is

$$|R(\omega)| \approx \sqrt{\frac{\kappa_1}{\kappa_0}} \left(1 - \left(\frac{\kappa'}{4\sqrt{2\rho c \kappa_0}} \right) \frac{1}{\sqrt{\omega}} + \dots \right) \quad (14)$$

Using three sufficiently high frequencies, the coefficients in eq.(14) can be found by linear regression. The frequencies are to be high enough such that the corresponding thermal wave will hardly penetrate beyond d. The foreknowledge of one of the conductivities allows one to select good frequency values. Up till here, we follow the same path as in ref.[5]. But here we note that, when the experimental data are poor, especially the linear term which we did use to obtain d can get less reliable. Therefore we now only use the constant term, which proved to suffer less from experimental errors, to obtain κ_0 . We then still need a procedure to determine d. We suggest the following. Measure |R| at a few lower frequencies for which the wave penetrates beyond the surface zone. Then choose a trial depth d_t and for this value calculate expression (13) at a few frequencies. Then one immediately can determine the frequency mismatch. If the theoretical frequency scale exceeds the experimental one by the factor a^2 , then we deduce from our invariance result that $d=ad_t$. This procedure is not much influenced by noise.

As an example Fig.1 shows the results of our procedure applied to a parabolic profile, for which we simulated three high-frequency |R|-values in a multilayer approach. We remark that our linear profile very well indicates the behavior of the actual profile. We note that in this particular case we also used the procedure of ref.[5] and arrived at good agreement. Fig. 2 shows how well the |R|-values of the parabolic and the linear profile resemble.

Fig.1 A parabolic conductivity profile and its obtained linear counterpart

Fig.2 The IRI-values for the two profiles of fig.1 can hardly be discriminated

In ref.[7] Ma et al. have used Mandelis' theory [4] to investigate surface-hardened steel. We have applied our method to their experimental results and arrive at a profile that closely matches theirs.

3.CONCLUSION

We have designed a method to investigate materials with inhomogeneous thermal conductivity within the surface region. It can be complementary to a related procedure that we have designed in the past. In particular it can serve as a check of that procedure when the available experimental high frequency data are of questionable quality. A few more experimental data are needed at any site under investigation and therefore the method is a little more time-consuming.

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