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TECHNICAL NOTES

Using the least square method for data reduction in the flash method

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INTRODUCTION

THE LASER flash method for thermal diffusivity measurements [1] is widely employed by scientists working in this field. In this method the front surface of a small disc-shaped sample receives a pulse of radiant energy from a laser and the thermal diffusivity value is computed from the resulting temperature response on the opposite surface of the sample. In an ideal case, when the sample is thermally insulated, initially at constant (zero) temperature, and the pulse is uniform and instantaneous, then the temperature rise vs time of the sample is given by the well-known formula [1]:

$$V(L,t) = B\left[1+2\sum_{n=1}^{\infty}(-1)^n \exp\left(-\frac{n^2\pi^2 at}{L^2}\right)\right] \quad (1)$$

where a is the thermal diffusivity, t the time, L the sample thickness and B the steady state temperature of the sample after the pulse. In what follows we will call this method the rear-face flash method.

In the front-face flash method (pulsed photothermal radiometry) [2–4], the temperature vs time history after the pulse is monitored on the front (irradiated) surface of the sample. With the same initial conditions as in the rear-face flash method, the temperature decay of the front surface following the pulse is

$$V(0,t) = B\left[1+2\sum_{n=1}^{\infty}\exp\left(-\frac{n^2\pi^2 at}{L^2}\right)\right]. \quad (2)$$

The desired parameters a and B in both methods can be determined by fitting the experimentally obtained curve to the corresponding theoretical one given by equations (1) and (2), respectively.

In the rear-face flash method, as is proposed in the original work [1], the thermal diffusivity can be calculated according to the formula

$$a = 0.139\frac{L^2}{t_{1/2}} \quad (3)$$

where $t_{1/2}$ is the experimentally obtained half-time, i.e. that time which corresponds to a rise in the temperature to half of its maximum value.

Results of such data reduction methods, which take into account one or several points from the experimental curves (e.g. refs. [5–7]), are very sensitive to distortions in the ideal curve given by equation (1). This is a consequence of the difficulties connected with the ideal conditions needed for the correct application of equation (1) or (2). In real experiments there is some heat loss in the sample, the pulse has finite duration, the heating of the sample is non-uniform, and the thermal properties vary with the temperature.

Using microcomputers and other modern means of data acquisition and data reduction make it possible to utilize the whole part of the experimental curve for evaluation of the desired thermal diffusivity. In order to avoid the effect of the above mentioned disturbing phenomena, especially the heat losses of the sample, new efficient data reduction methods have recently appeared considering the entire experimental curve, and more particularly its rising part [8–10]. A survey of existing methods can be found in ref. [11].

In addition, experimental curves are distorted from low frequency noise of the temperature vs time signal. In order to remove this effect in the rear-face flash method, Pawlowski and Fouchais [12] suggested the least square fitting technique, which is based on numerical minimization of the function

$$R(a,B) = \sum_{i=1}^{N}[U_i - V(L,t_i)]^2 \quad (4)$$

where U_i are the experimentally acquired data corresponding to the time point t_i, and $V(L,t_i)$ are the values given by equation (1). N is the number of experimental points taken into account. These authors determined the minimum of the function (4) by using the iterative procedure proposed in ref. [16].

For the calculation of the theoretical temperature rise $V(L,t)$ or $V(0,t)$ at relatively small times after the pulse (in transient area), however, it is better to use the formulae derived from the general equation given in ref. [13]

$$V(L,t) = B\frac{2L}{\sqrt{(\pi at)}}\left[\sum_{n=0}^{\infty}\exp\left(\frac{-(2n+1)^2L^2}{4at}\right)\right] \quad (5)$$

and

$$V(0,t) = B\frac{L}{\sqrt{(\pi at)}}\left[1+2\sum_{n=1}^{\infty}\exp\left(-\frac{n^2L^2}{at}\right)\right] \quad (6)$$

for the front-face flash method. These series converge quite rapidly except for large values of at/L^2. Therefore in the same sense they represent the complementary formulae to equation (4) or (2), respectively, which are more convergent for large values of time. The reason for the application of equations (5) and (6) instead of equations (1) and (2) is due to the fact that the experimental data for the smaller times after the pulse are less affected by heat loss from the sample. This is why the diffusivity must be identified as soon as possible during the experiment [9, 14].

The purpose of this note is to describe an improved algorithm for data reduction in the rear-face and front-face flash methods using the least square technique, in which the experimental data are fitted to the theoretical values according to equations (5) and (6), respectively. The minimum of the least square function (4) is determined by means of mainly analytical methods. Though the formulae used ignore the heat loss from the sample, in what follows it is shown that our technique leads to diffusivity determination of equivalent accuracy as in the other existing methods with the heat loss correction.

NOMENCLATURE

a	thermal diffusivity	t	time
a^*	optimal value of thermal diffusivity	$t_{1/2}$	half time
B	maximum temperature rise	U_i	experimental data
L	sample thickness	V	theoretical temperature.
N	number of points taken into computation		

FORMULATION

We seek the minimum of the least square function

$$R(a,B)=\sum_{i=1}^{N}\left\{U_i-B\frac{2L}{\sqrt{(\pi a t_i)}}\sum_{n=0}^{\infty}\exp\left(\frac{-(2n+1)^2L^2}{4at_i}\right)\right\}^2 \tag{7}$$

or

$$R(a,B)=\sum_{i=1}^{N}\left\{U_i-B\frac{L}{\sqrt{(\pi a t_i)}}\left[1+2\sum_{n=0}^{\infty}\exp\left(-\frac{n^2L^2}{at_i}\right)\right]\right\}^2 \tag{8}$$

for the front-face flash method. Here a and B are the parameters to be estimated. The necessary conditions for the extremes of $R(a,B)$ are given by the following equations:

$$\frac{\partial R(a,B)}{\partial a}=0;\quad \frac{\partial R(a,B)}{\partial B}=0. \tag{9}$$

Performing the indicated operations, and after a lengthy but straightforward set of manipulations, the equations for a and B obtain the form

$$\sum_{i=1}^{N}U_iT_i(a)\sum_{i=1}^{N}T_i(a)\frac{\partial T_i(a)}{\partial a}-\sum_{i=1}^{N}U_i\frac{\partial T_i(a)}{\partial a}\sum_{i=1}^{N}T_i^2(a)=0 \tag{10}$$

$$B=\sum_{i=1}^{N}U_iT_i(a)\left(\sum_{i=1}^{N}T_i^2(a)\right)^{-1} \tag{11}$$

where

$$T_i(a)=\frac{2}{\sqrt{t_i}}\sum_{n=0}^{\infty}\exp\left(-\frac{(2n+1)^2L^2}{4at_i}\right) \tag{12}$$

in the rear-face method, or

$$T_i(a)=\frac{1}{\sqrt{t_i}}\left[1+2\sum_{n=1}^{\infty}\exp\left(-\frac{n^2L^2}{at_i}\right)\right] \tag{13}$$

in the front-face method.

Let us remark here that in a similar way one can derive the formulae for a and B from equations (1) and (2), respectively. In that case they turn out to be

$$\sum_{i=1}^{N}U_iS_i(a)\sum_{i=1}^{N}S_i(a)\frac{\partial S_i(a)}{\partial a}-\sum_{i=1}^{N}U_i\frac{\partial S_i(a)}{\partial a}\sum_{i=1}^{N}S_i^2(a)=0 \tag{14}$$

$$B=\sum_{i=1}^{N}U_iS_i(a)\left(\sum_{i=1}^{N}S_i^2(a)\right)^{-1} \tag{15}$$

where

$$S_i(a)=\left[1+2\sum_{n=1}^{\infty}(-1)^n\exp\left(-\frac{n^2\pi^2at_i}{L^2}\right)\right] \tag{16}$$

in the rear-face method, or

$$S_i(a)=\left[1+2\sum_{n=1}^{\infty}\exp\left(-\frac{n^2\pi^2at_i}{L^2}\right)\right] \tag{17}$$

in the front-face method.

The desired optimal values of a and B are obtained as a solution to the equation system (10) and (11), where $T_i(a)$ is the relevant function given by either equation (12) or (13).

DISCUSSION

The problem of finding the optimal values of the parameters a and B is now reduced to solving equation (10) for a. Parameter B depends functionally on a (equation (11)). If we denote the left-hand side of equation (10) as $F(a)$, then, as we can see from Fig. 1, this function has only one simple root a^* (except for the trivial one in zero), which corresponds to the desired optimal value of the thermal diffusivity. For all $a > a^*$ and $0 < a < a^*$, $F(a) > 0$ and $F(a) < 0$, respectively. This fact facilitates the procedure of computation of a from equation (10) by means of any of the standard numerical methods.

To demonstrate the use of this data reduction method in the rear-face flash method, for a sample with heat losses, we present in what follows the results obtained from the measurements of the thermal diffusivity of an oxide ceramic sample of composition $YBa_2Cu_3O_{7-\delta}$, and the sample from glass. Both samples from low-diffusivity materials had the form of a circular cylinder, whose radius was about 4 mm, and height $L = 3$ mm for the ceramic and $L = 4.730$ mm for the glass sample. The mean temperature of the ceramic sample during the experiment was 401°C, and for the glass sample it was 27°C. The flash was generated by a xenon-flash lamp. We have assumed that the effects of finite duration of the pulse and non-uniform heating of the sample were negligibly small.

In accord with the above mentioned fact, we have taken into account the experimental points which lie in the first third of the rising part of the temperature vs time curve. Except for the part lying immediately behind the pulse, which is distorted by electrical interaction of the data acquisition system with the pulse generator and whose points have small weight [9], we took into account 40–80 experimental points. A comparison of our results with the results determined by other methods is given in Table 1, and shows that the present method of data reduction is comparable in accuracy with other special methods [8–10].

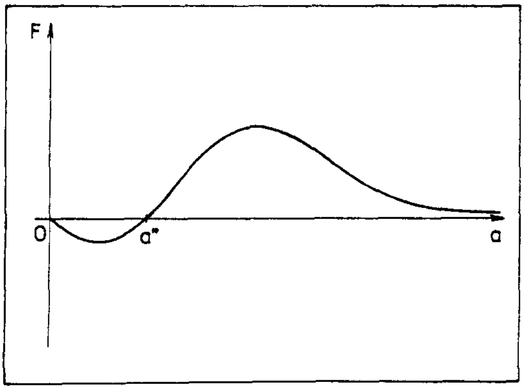

FIG. 1. Function F vs a.

Table 1. Results of data reduction

Method		Ceramic		Glass	
		a (10^7 m^2 s^{-1})	B	a (10^7 m^2 s^{-1})	B
Parker *et al.* [1]		5.296	163	5.321	187
Degiovanni [8]	($a_{1\ 3}$)	3.930		4.599	
	($a_{1\ 2}$)	3.845		4.559	
	($a_{5\ 6}$)	3.760		4.435	
Balageas [9]		4.018	266	4.555	236
Degiovanni and Laurent [10]		3.849		4.405	
Present work		3.989	258	4.481	257

If it is necessary to take into account the correction due to the duration and shape of the heat pulse, then the procedure of Azumi and Takahashi [15] must be used first, for the time origin calculation.

The time necessary to fit one set of experimental data on a personal computer varies from 4 to 12 min, and depends on the number N of the experimental points (40–200), which were taken into the computation, as well as on the required precision of the results.

The application of formulae (5) and (6), which converge more rapidly for small times than those given in ref. [12], and the determination of the minimum of the least square function by a mainly analytical method, means that our algorithm is simpler and faster than that described in ref. [12].

In comparison with other methods [8–10] our procedure, apart from its physical simplicity, can be applied to a very noisy signal.

The large field of application of this procedure is in the front-face flash method, which seems to be a promising tool for remote, non-destructive measurements of the thermal properties of surfaces. Early stages of the transient area after a heat pulse contain less affected information about thermophysical parameters of the sample, the values of which can be determined from the temperature vs time curves by using the least square method.

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