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TRANSIENT THERMAL MODELLING OF LAYERED MATERIALS. CRITICISM OF FOURIEREAN THEORY WITH RESPECT TO THE SPEED OF HEAT PROPAGATION

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It is well known that the imposing of boundary conditions (BC) at the outer sample boundaries leads to an infinite speed of propagation of heat. Although any finite temperature difference is propagated with a finite velocity, the temperature history at a given point does not in general reflect the correct layer sequence. In order to overcome this non-physical description, we treat two simple examples as Stefan problems (moving BC at the propagation front).

Thermal investigations of layered materials have been applied successfully to the evaluation of a wide range of materials, such as thin films (coatings) [1, 2], semiconductor devices [3–6] and even living human skin [2]. They provide a powerful tool for non-destructive material testing and for semiconductor engineering, an interesting supplement and/or alternative for electrical and optical measurements.

In semiconductor injection laser diodes, heat can be generated by current through the *pn* junction, while the heat transfer is detected via the temperature-dependence of the junction voltage drop [4, 5, 7]. In recent measurements [4, 5], characteristic structures of this temperature history have been observed, which are empirically connected with the crossing of an interface by the heat propagation front.

On the other hand, the theoretical modelling, e.g. [2, 6, 8], uses the classical diffusion theory of Fourier [9], which deals with spatial diffusion modes extending over the whole sample. It is well known that the distant boundary conditions (BC) at the sample boundaries imply an infinite speed of heat propagation (in order to "feel" them instantaneously at the heat source). And although the spatial heat propagation can be recovered by the temperature rise after power supply at

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different loci in the sample [10], the temperature history at the source will, in general, not reflect the proper layer sequence in multilayer stacks. This is exemplified in the following section.

Therefore, we shall show that the terms in the Fourier series often do not sum up to the correct heat propagation through layer by layer; in other words, the diffusion modes (reflecting collective stack properties) do not superpose to the physically correct picture of a moving front of propagation [6, 11].

Consequently, this front of propagation has to be imposed from the very beginning, i.e. via a moving BC, as in the Stefan problems [12]. In this paper, we consider the linear single-layer and the two-layer problem, with special attention to cusp-like structures in the surface temperature history and applying the heat-balance integral method [13]. Throughout, we assume the quasi-one-dimensionality of heat transfer.

The failure of Fourierean diffusion theory

Let us consider a stack of 8 homogeneous layers, the data on which are listed in Table 1, without interface resistances. Heat is supplied by a Dirac pulse of energy flux density Q_{s0} on the surface of layer 1 ($x=0$). The rear surface (layer 8) is thermally isolated. Thus, we imagine pulsed photothermal inspection of this GaAlAs chip.

We have calculated [6] the apparent effusivity [2]

$$e(t) = Q_{s0}/T(0, t)\sqrt{\pi t} \tag{1}$$

because this displays much more pronounced structures than the surface temperature history, $T(0, t)$, itself [6] (cf. [2], Figs 9 and 10). The result is shown in Fig. 1. More than 3000 terms are included in the Fourier series (the solution of the

Table 1 Material constants of the eight-layer model [6]

i, layer	d_i, 10^{-6} m	$\varkappa_i$, 10^{-6} m^2 s^{-1}	k_i, Wm^{-1} deg^{-1}
1	90	23.7	41.5
2	2	7.06	12
3	0.2	11.6	20
4	1.3	7.06	12
5	0.8	23.7	41.5
6	0.2	5.0	10
7	0.7	33.3	100
8	11	15	26

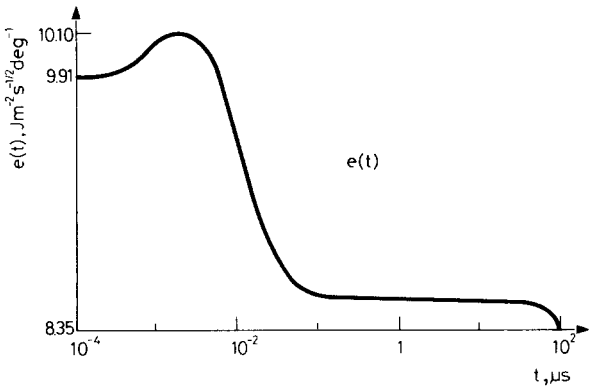

Fig. 1 Apparent effusivity for the eight-layer stack [6]

transcendent eigenvalue equation for the decay constants of the diffusion modes was circumvented by employing their asymptotic behaviour [6, 14]). The plateau of $e(t)$ below $t \sim 0.1$ ns was achieved, which proves the convergence of the series used.

However, the first deviation from this plateau (representing the behaviour of a homogeneous semi-infinite probe [2]) stems not from the second layer of the stack, but from the third one. Generally, it can be shown [14] that it arises from the layer with the smallest value of $\eta_i = d_i/\varkappa_i^{1/2}$, where d_i and $\varkappa_i$ are the thickness and the thermal diffusivity of the i-th layer, respectively. And this is independent of the position of this layer within the stack! This is the main reason for our criticism of distant BC for general multilayer systems.

Correspondingly, the temperature *vs.* time curve at the *pn* junction (electrical heating) calculated in this way [6, 11] does not obey the cusp-like structures observed experimentally [4, 5]. Similarly, the experimental surface temperature history of the three-layer model (living human skin) in [2], when appropriately redrawn in a log-log scale, shows much sharper structures than the theoretical curve (cf. Fig. 9 in [2]) [5].

Moving boundary condition. Single-layer case

Let us consider the following problem:

$$T_t(x, t) = \varkappa T_{xx}(x, t), \qquad 0 \leqslant x \leqslant d \tag{2}$$

$$T(x, 0) = 0, \qquad 0 \leqslant x \leqslant d \tag{3}$$

$$T_x(0, t) = -f = \text{const} < 0 \tag{4}$$

$$T(x, t) = 0, \qquad x_0(t) \leqslant x \leqslant d \tag{5}$$

$$-\varkappa T_x(x_0, t) = \dot{x}_0 T(x_0, t) \tag{6}$$

$$T_x(x_0, t) = 0 \tag{7}$$

$$T_{xx}(x_0, t) = 0 \tag{8}$$

$0 \leqslant t \leqslant t_1$. Here, $x_0(t)$ is the position of the propagation front (penetration distance) at time t, $x_0(0) = 0 \leqslant x_0(t) \leqslant d = x_0(t_1)$. $T_t = \partial T/\partial t$, etc., $\dot{x}_0 = \mathrm{d}x_0/\mathrm{d}t$. (6) expresses the moving BC and guarantees the total energy conservations. (7) follows from (5) and (6). The smoothness condition (8) is derived by differentiation of (5) with respect to time and using (2) and (7) [13].

Equations (2) to (8) describe the first stage, $0 \leqslant t \leqslant t_1$, where the heat supplied at $x=0$ moves to the rear surface at $x=d$; but $T(x, t) = 0$ for $x \geqslant x_0(t)$, the rear surface is not "felt", and the problem is that of a semi-infinite sample.

Following Goodman [13], we solve it approximately by means of the heat-balance integral,

$$\int_0^{x_0} T_t(x, t)\,\mathrm{d}x = \frac{d}{\mathrm{d}t}\int_0^{x_0} T(x, t)\,\mathrm{d}x = \varkappa \int_0^{x_0} T_{xx}(x, t)\,\mathrm{d}x = \varkappa f \tag{9}$$

which replaces the local balance relation (2) by the global one; the former will therefore be fulfilled only on average.

A reasonable approximation is the cubic profile

$$T(x, t) = \frac{f}{3} x_0(t)[1 - x/x_0(t)]^3 \tag{10}$$

satisfying (3) to (5), (7) and (8). Inserting (10) into (9) yields

$$x_0(t) = \sqrt{12\varkappa t}, \qquad 0 \leqslant t \leqslant t_1 \tag{11}$$

and

$$t_1 = d^2/12\varkappa \tag{12}$$

The surface temperature increases according to

$$T(0, t) = x_0(t) f/3 = 2f\sqrt{\varkappa t/3} \tag{13}$$

As noted by Goodman [13], the factor $2/\sqrt{3}$ differs by only 2% from the "exact" one, $2/\sqrt{\pi}$, of the "classical" result for $T(0, t)$. The latter, however, imposes the distant BC $T(\infty, t) = 0$, and not (5) (which is indeed not fulfilled by it), and is therefore not an exact measure of comparison.

In the second stage, $t \geqslant t_1$, $x_0(t)$ stays at d, where we assume the isothermal BC

$$T(d, t) = 0 \tag{14}$$

and Eqs (2) to (9), except (7), remain valid, replacing x_0 by 1. The corresponding cubic temperature profile is then [13]

$$T(x, t) = \frac{1}{2}[3T(0, t) - fd]\left(1 - \frac{x}{d}\right) + \frac{1}{2}[fd - T(0, t)]\left(1 - \frac{x}{d}\right)^3 \tag{15}$$

$$T(0, t) = fd\left(1 - \frac{2}{3}\exp\{-(t - t_1)/5t_1\}\right), \qquad t \geqslant t_1 \tag{16}$$

Formula (16) approximates the first two terms of the corresponding Fourier series with the correct values for $t = t_1$ and $t = \infty$, cf. [10].

According to (13) and (16), we obtain an angle in the $T(0, t)$ curve at $t = t_1$, since

$$T_t(0, t_1 - 0) = 2\frac{f\varkappa}{d} > T_1(0, t_1 + 0) = 1.6\frac{f\varkappa}{d} \tag{17}$$

Of course, both numerical values are approximative ones, but it is obvious that the shape of the curve $T(0, t)$ must change at $t = t_1$, namely from the square-root increase (13) to a saturation-like one (16). This behaviour is more pronounced when the concept of penetration distance (moving BC) is used for the first stage. Moreover, the correlation between the spatial and temporal particularities is guaranteed by the construction.

Moving boundary condition. Two layers

Let us now study the effet of a heterointerface (without thermal resistance). During the penetration of heat into the first layer (first stage), the problem is identical to the single-layer case (all parameters will be labelled by 1).

When $t = t_1$, $x_0(t_1) = d_1$, the propagation front crosses the interface and changes its penetration law. We describe this second stage by means of the heat-balance integral method [13], too.

Since the choice of the approximative temperature profile is not unique, we must proceed intuitively, guided by physical requirements such as the continuity of temperature and heat flow at the interface:

$$T_1(d_1, t) = T_2(d_1, t) \tag{18}$$

$$k_1 T_{1x}(d_1, t) = k_2 T_{2x}(d_1, t) \tag{19}$$

where k is the heat conductivity. Furthermore, the solution for the second stage should go over into that for the first one if the material constants of the two layers are the same.

A simple ansatz to satisfy all this is (cf. Fig. 2)

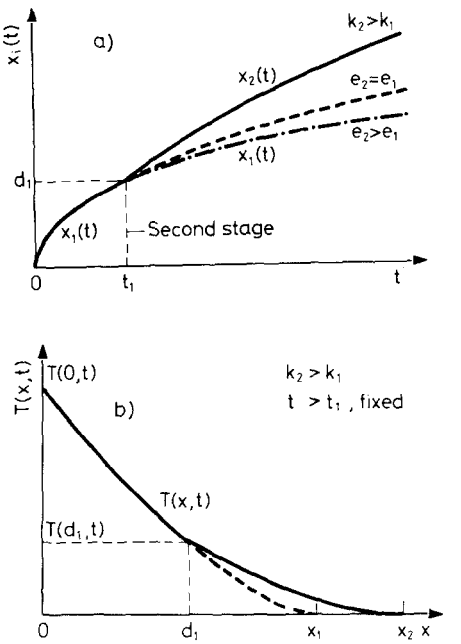

Fig. 2 a) Penetration distances during the second stage: the apparent one for the first layer, $x_1(t)$, and the true one, $x_2(t)$; b) cubic temperature profiles for the second stage

$$T(x,t) = \frac{1}{3} f d_1 \begin{cases} A(t)(1-x/x_1(t))^3, \\ B(t)(1-x/x_2(t))^3, \end{cases} \quad x \lesseqgtr d_1 \tag{20}$$

Inserting (20) into (4), (18) and (19), we get

$$A(t) = x_1(t)/d_1 \tag{21}$$

$$B(t) = A(t)(1-d_1/x_1)^3/(1-d_1/x_2)^3 \tag{22}$$

$$B(t) = A(t)k_1x_2(1-d_1/x_1)^2/k_2x_1(1-d_1/x_2)^2 \tag{23}$$

Hence,

$$\frac{k_1}{k_2}\left(\frac{x_2}{d_1}-1\right) = \frac{x_1}{d_1}-1 \tag{24}$$

The fourth relation needed is provided by the heat-balance integral

$$p_1 \int_0^{d_1} T_t(x, t)\,\mathrm{d}x + p_2 \int_{d_1}^{x_2} T_t(x, t)\,\mathrm{d}x = k_1 f \tag{25}$$

where $p = k/\varkappa$ denotes the heat capacity per volume and (4), (7) and (19) have been used. With (20) to (24), this gives

$$\frac{x_1^2}{d_1^2}\left[1 + \left(\frac{e_2^2}{e_1^2} - 1\right)\left(1 - \frac{d_1}{x_1}\right)^4\right] = \frac{12\varkappa_1 t}{d_1^2} = \frac{12t}{T_1}, \qquad T_1 = d_1^2/\varkappa_1 \tag{26}$$

where $e_i = \sqrt{k_i p_i}$ is the material effusivity. For $e_1 = e_2$, formula (26) goes over into (11), as required; for $x_2 = x_1 (= x_0(t))$, $k_2 = k_1$ is also necessary, see (24).

Stage 2 lasts from t_1 to t_2, defined by $x_2(t_2) = d = d_1 + d_2$ and calculated via (26) from $x_1(t_2)$, given through (24) as

$$\frac{x_1(t_2)}{d_1} = 1 + \frac{k_1}{k_2}\left(\frac{d}{d_1} - 1\right) \tag{27}$$

The surface temperature history is described by

$$T(0, t) = \frac{f}{3} x_1(t), \quad t_1 \leqslant t \leqslant t_2, \quad x_1(t_1) = x_0(t_1) = d_1 \tag{28}$$

Hence, its smoothness at $t = t_1$ is determined by that of $x_{1(0)}$. From (26) it follows that

$$\dot{x}_0(t_1) = \dot{x}_1(t_1) \tag{29}$$

Though the time-dependence of the penetration distance changes. Consequently,

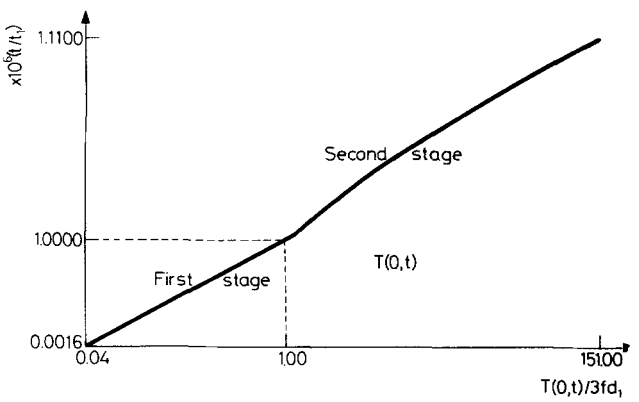

Fig. 3 Surface temperature history, Eqs (13) and (28). $d_2 = 30d_1 = 3$ mm, $k_2 = 5k_1 = 70$ W/deg m, $p_2 = p_1 = 3.9$ J/deg cm^3, $t_1 = 4.64 \times 10^{-5}$ s (Ni–Cr on steel, cf. [2])

within this approximation, the interface crossing of the propagation front does not cause a sharp structure (angle) in $T(0, t)$, see fig. 3.

If $e_2 > e_1$, $T(0, t)$ will rise more slowly for $t \geqslant t_1$ than for $t \leqslant t_1$, since relatively more heat is conducted into layer 2, and vice versa. It is remakable that, within the present approximation, the interface crossing is not reflected in $T(0, t)$, if $p_2 \neq p_1$ and $k_2 \neq k_1$, but $p_2 k_2 = p_1 k_1$ ("degeneracy").

Conclusions

We have demonstrated that the "classical" Fourierean diffusion theory working with diffusion modes extended over the whole sample is, in general, not able to reflect the actual layer sequence in the surface temperature history. Consequently, a correct interpretation of photothermal data, for example, is possible only in some special cases.

On the other hand, the concept of penetration distance leads to solutions which incorporate by construction a front of heat propagation. Consequently, the surface temperature history displays structures, the temporal sequence of which is immediately related to the layer sequence of the stack under consideration.

The heat-balance integral method seems to provide a useful tool for solving this Stefan-like problem for multilayer systems, too, but eventually more sophisticated trial profiles than (20) are in order for higher accuracy, cf. [13].

When heat is generated within the sample, as, for example, in laser diodes, "interference" effects from interface crossings in opposite directions should occur. Further complications arise when the heat transfer is essentially more-dimensional [13].

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References

1 P. Cielo, J. Appl. Phys., 56 (1984) 230.
2 D. L. Balageas, J. C. Krapez and P. Cielo, ibid., 59 (1986) 348.
3 S. J. SHeard, R. K. Appel and M. G. Somekh, Electron. Lett., 23 (1987) 227.
4 J. J. Hughes, D. G. Gilbert and F. Z. Hawrylo, RCA Review, 46 (1985) 200.
5 W. Both, unpublished
6 J. Galley and P. Enders, Heat Transfer in Multilayer Systems. Limits of "Classical" Diffusion Theory, ZOS–Preprint, Berlin 1987.
7 T. Szirányi, Int. J. Electronics, 63 (1987) 153.

8 W. Nakwaski, IEE Proc., Pt. I., 131 (1984) 94.
9 J. B. Fourier, La théorie de la chaleur, Gauthier–Villars, Paris 1822.
10 H. Tautz, Wärmeleitung und Temperaturausgleich, Akademie–Verlag, Berlin 1971.
11 P. Enders and J. Galley, Proc. Int. Conf. Semiconductor Injection Lasers SELCO '87, Oct. 11–16, 1987, Holzhau (G.D.R.), to be published in Soviet Phys. – Quantum Electron. (1988).
12 L. I. Rubinshtei'n, Problema Stefana, "Zwai'gzne", Riga 1967.
13 T. R. Goodman, in: Adv. Heat Transfer (T. F. Irvine and J. P. Hartnett, Eds.0, Vol. 1, Academic Press, New York/London 1964, p. 51.
14 P. Enders, J. Thermal Anal., 34 (1988) 319.

Zusammenfassung — Wie bekannt, hat die Festlegung von Randbedingungen (BC) an den äusseren Grenzen einer Probe eine unendliche Wärmeausbreitungsgeschwindigkeit zur Folge. Obwohl sich jeglicher endlicher Temperaturunterschied mit endlicher Geschwindigkeit ausbreitet, spiegelt der Temperaturverlauf an einem gegebenen Ort im allgemeinen die korrekte Schichtensequenz nicht wider. Zur Ausmerzung dieser unphysikalischen Beschreibung wurden zwei einfache Beispiele als Stefan-Problem (bewegliche BC an der Ausbreitungsfront) behandelt.

Резюме — Хорошо известно, что наложение граничных условий на внешние границы раздела образца приводит к бесконечной скорости распространения тепла. Хотя какое-либо тепловое различие распространяется с конечной скоростью, тепловое происхождение при данной точке, в общем, не отражает истинную последовательность слоя. Во избежание этого не физического описания, авторы провели обработку двух простых примеров в виде задачи Стефана (движение граничных условий во фронте распространения).