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HEAT CONDUCTION IN MULTILAYER SYSTEMS

Asymptotics of Temperature Decay Constants

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For linear Fourierian, quasi-one-dimensional heat conduction in a stack of homogeneous layers, it is shown that the temperature decay constants, τ_n, behave asymptotically as n^{-2}. This yields a considerable lowering of computer time at a satisfactory accuracy level. A numerical example is given. The matching problem of the alternative infinite series containing terms such as $e^{-t/\tau}$ and $e^{-a/t}$, respectively, is also considered, and the equivalence between surface excitation and a volume excitation is demonstrated.

The temporal and spatial temperature behaviour after the pulsed or step-like excitation of layered materials contains useful information on the thermophysical material properties, as well as on the presence of subsurface defects or delaminations, on the interface quality, etc. [1]. In semiconductor device analysis, it provides interesting alternatives to electrical and optical investigations [2], and it is important for the laser heating of slabs [3].

Experimentally, one may excite the surface with a flash lamp or laser beam and observe the temperature of the rear-face or of the front surface (pulsed photothermal inspection [1]. In bipolar semiconductor devices, heat is generated mainly at the $p-n$ junction, which leads to a similar temperature history [2].

Mathematically, one has to solve the heat diffusion equation in each layer and to match the solutions at the interfaces (we will not consider a moving boundary condition; see [3] and references (therein). Although one can always apply numerical methods (this will be necessary when the temperature-dependence of the material constants comes into play and variational methods are not applicable), analytical solutions are preferable, as they provide more insight into many details of the processes involved.

Analytical solutions of the linear heat diffusion equation in one to three spatial dimensions for a stack of N homogeneous layers (or even more complicated compositions, when only the interfaces are rectangular to each other) can be

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obtained by standard methods (e.g. [1, 2] and references therein). Within Fourier's method of separation of variables, one obtains an infinite series of exponential decay terms (after Dirac pulse excitation):

$$\theta(x, t) = \sum_{n=0}^{\infty} F_n(x) e^{-t/\tau_n} \tag{1}$$

(in one dimension, to which we confine ourself in this paper), with prefactors $F_n(x)$ and decay constants τ_n, depending upon the boundary conditions at the interfaces and sample surfaces, as well as upon the excitation location. (The infinitely many pictures in two confronted mirrors comprise an optical analogue to this series [4]).

The decay constants are the reciprocal eigenvalues of a Sturm–Liouville operator and form an infinite sequence of decreasing values with limit zero (cf. below); the number of trigonometric terms in the transcendent eigenvalue equation increases as 2^N [2]. The Fourier analysis in terms of diffusion modes is in general *an*harmonic [4].

Consequently, the number of terms in (1) to be accounted for increases rapidly with decreasing time interval between excitation and observation. On the other hand, the alternative expansion of $\theta(x, t)$ with respect to terms such as $e^{-a/t}$ [5] may converge well only for very short times (cf. below).

Thus, the goal of this paper is twofold. First, in section 1, we derive our observation $\tau_n \sim n^{-2}$ as $n \to \infty$ [6], providing a useful tool for calculating high-n terms in (1) *without* solving the eigenvalue equation. Secondly, in section 2, we consider the asymptotic behaviour of temperature and effusivity for small and large times, and attempt to connect the two series mentioned above, i.e. to estimate a cut-off time t_c, above which (1) is more useful, while below it the other series is better. Finally, section 3 presents some numerical results and summarizes this paper.

For the sake of simplicity and comparison with [1], our concrete calculations concern the front-surface temperature monitoring of quasi-one-dimensional two- and three-layer materials with perfect interfaces, but the generalization to other cases is straightforward (in order to apply Fourier's method of separation of variables directly in the case of surface excitation, we show in Appendix A how the latter can be converted into a "volume" excitation).

1. Asymptotics of temporal decay constants

Let us consider a quasi-one-dimensional stack of N homogeneous layers with temperature-independent thermal coefficients. Let heat be generated by absorption of a Dirac pulse of heat flux onto one end of the stack, while the other end is thermally isolated. The interfaces may have no thermal resistance. (For a discussion of these simplifying assumptions, cf. [2, 7].

Then, for the whole stack we have the diffusion equation for the temperature:

$$\dot{\theta}(x, t) = \frac{1}{\varrho c}(K\theta')' + Q\delta(x)\delta(t) \tag{2}$$

($\dot{} = \partial/\partial t$, $' = \partial/\partial x$), where the density ϱ, heat capacity c and thermal conductivity K are step-wise constants. The surface excitation is converted into a volume term (see Appendix A). Separation of variables, $\theta(x, t) = X(x)T(t)$, leads to

$$\frac{\dot{T}}{T} = \frac{1}{\varrho c X}(KX')' = \text{const} = -\frac{1}{\tau} \tag{3}$$

and thus to $T(t) = e^{-t/\tau}$ (the integration constant can be incorporated into $X(x)$. and to the Sturm–Liouville eigenvalue problem [8]:

$$-\frac{1}{\varrho c}(KX')' = \frac{1}{\tau}X(x) \tag{4a}$$

$$X'(0) = X'(L) = 0 \tag{4b}$$

Now the asymptotics of eigenvalues $1/\tau$ is well known when the coefficient of X'' is constant [8]. This can be achieved by the Sturm–Liouville transformation, which requires, however, that the coefficients in (4a) are twice continuously differentable. However, this condition can be weakened if the first derivative is retained after transformation ($H = 1$ in [8], p. 61) Let

$$\xi = h(x), \quad X(x) = \Xi(\xi). \tag{5}$$

Then, (4a) becomes

$$\frac{1}{\varrho c}[-\Xi'' K h'^2 - (Kh')'(\Xi' + \Xi)] = \frac{1}{\tau}\Xi \tag{6}$$

Obviously, the coefficient of Ξ'' becomes -1 when

$$h(x) = \int_0^x \sqrt{\frac{\varrho c}{K}}\,dx' = \int_0^x \frac{dx'}{\sqrt{\varkappa(x')}} \tag{7}$$

where $\varkappa = K/\varrho c$ is the (temperature) diffusivity.

Finally,

$$-\Xi'' - \frac{de}{dx}(h^{-1}(\xi))(\Xi' + \Xi) = \frac{1}{\tau}\Xi \tag{8}$$

where $e = \sqrt{K\varrho c}$ is the effusivity.

The stack total length L is transformed to the ξ-interval $[h(0), h(L)]$, i.e.

$$L_\xi = h(\mathrm{L}) - h(0) = \int_0^L \frac{dx}{\sqrt{\varkappa}} = \sum_{i=1}^{N} \frac{L_i}{\sqrt{\varkappa_i}} \equiv \sum_{i=1}^{N} \eta_i = \eta \tag{9}$$

Thus, the asymptotic behaviour of the decay constants [8] is given by

$$\frac{1}{\tau_n} \to \left(\frac{n\pi}{\eta}\right)^2 \quad \text{as} \quad n \to \infty \tag{10}$$

This is the desired relation. We have observed it for the three-layer model (living human skin) in [1], for which $\tau_n = \eta_3^2/\gamma_n^2$, and hence

$$\gamma_n \to n\pi/\omega_1 = 2.92n \quad (\omega_1 = \eta_1/\eta_3 + \eta_2/\eta_3 + 1) \tag{11}$$

The physical background of this asymptotics is simple: with increasing order n, the spatial variation of the diffusion modes becomes faster and faster (increasing number of nodes, i.e. zeros of $F_n(x)$ in (1); and the nature of diffusion will be dominated by these volume variations against those imposed by the boundary conditions. In other words, the Fourier series becomes increasingly harmonic (cf. [4, 8]).

It is worth noting, however, that there remains a finite difference between the exact eigenvalues and their asymptotic values (10) (see Appendis B). Since the prefactors in (1) react quite sensitively to slight changes in τ_n (cf. Table 2 below), the application of this asymptotics has to be done with care.

2. Temperature behaviour for very small and very long times.
Series cut-off and matching

For a two-layer system, the Laplace-transformed solution of (4) for the front-surface temperature ($x=0$) reads

$$\bar{\theta}_2(s) = \frac{1}{e_1\sqrt{s}} \cdot \frac{x_1 ch(\omega_1\eta_2\sqrt{s}) + x_2 ch(\omega_2\eta_2\sqrt{s})}{x_1 sh(\omega_1\eta_2\sqrt{s}) + x_2 sh(\omega_2\eta_2\sqrt{s})} \tag{12}$$

with

$$\begin{aligned} x_1 &= e_{12}+1, \quad & x_2 &= e_{12}-1, \quad & e_{12} &= e_1/e_2, \\ \omega_1 &= \eta_{12}+1, \quad & \omega_2 &= \eta_{12}-1, \quad & \eta_{12} &= \eta_1/\eta_2 \end{aligned} \tag{13}$$

(cf. Eq. (20) in [1] with $1/h = 0$). Hence [5]:

$$\lim_{t\to\infty} \theta_2(t) = \lim_{s\to 0} s\bar{\theta}_2(s) = 1/\sum_{i=1}^{2} \varrho_i c_i L_i \tag{14}$$

in agreement with Eq. (21) in [1]; because of the thermal isolation, (14) represents the uniform temperature rise per unit excitation strength after long times ($t \gg \tau_1$, where $\tau_1 = \eta_2^2/\gamma_1^2$ is the largest decay constant). Further,

$$\lim_{t\to 0} \theta_2(t) = \lim_{s\to\infty} s\bar{\theta}_2(s) \sim \lim_{s\to\infty} s^{1/2} = \infty \tag{15}$$

corresponding to the Dirac pulse shape of excitation.

For the apparent effusivity [1]:

$$e(t) = 1/\theta(t)\sqrt{\pi t} \quad (16\text{-}$$

we obtain

$$\lim_{t\to\infty} e(t) = 0 \tag{17}$$

$$\lim_{t\to 0} e(t) = e_1 \tag{18}$$

(applying (15) to $\theta_2(t)\sqrt{t}$ and using the convolution theorem [5]; cf. also the square-root behaviour in (15)).

It turns out that (18) is a convenient measure for testing the validity of cut-offs of (1), as well as that of applying (10); for small times, $e(t)$ must go over into a plateau (cf. Figs 4, 8, and 10 in [1], and below).

On the other hand, as pointed out by Balageas et al. [1], the number of terms needed in (1), n_{max}, increases rapidly with decreasing time values after excitation, t_{min}. In fact, Eq. (10) shows that the decay constants decrease rather slowly, and $t_{min} \gg \tau_{min}$ implies

$$n_{max} \gg \eta/\pi\sqrt{t_{min}} \tag{19}$$

For instance, the calculation of $e(t)$ for the three-layer model in [1] up to $t_{min} = 10^{-2}$ s requires more than 200 terms.

Here, it is favourable to use the alternative form of back transformation of (12):

$$\begin{aligned}\bar{\theta}_2(s) &= \frac{1}{e_1\sqrt{s}}[1 + x_{21}(e^{-2\eta_1\sqrt{s}} + e^{-2\eta_2\sqrt{s}}) + e^{-2(\eta_1+\eta_2)\sqrt{s}}]/ \\ &\quad [1 - x_{21}(e^{-2\eta_1\sqrt{s}} - e^{-2\eta_2\sqrt{s}}) - e^{-2(\eta_1+\eta_2)\sqrt{s}}] = \\ &= \frac{1}{e_1\sqrt{s}}[1 + x_{21}(e^{-2\eta_1\sqrt{s}} + e^{-2\eta_2\sqrt{s}}) + e^{-2(\eta_1+\eta_2)\sqrt{s}}] \\ &\quad X\sum_{n=0}^{\infty}[x_{21}(e^{-2\eta_1\sqrt{s}} - e^{-2\eta_2\sqrt{s}}) + e^{-2(\eta_1+\eta_2)\sqrt{s}}]^n\end{aligned} \tag{20}$$

with $x_{21} = x_2/x_1$ ($|x_{21}| < 1$). This series can be transformed term by term [5], giving

$$\theta_2(t) = \frac{1}{e_1\sqrt{\pi t}}(1 + 2x_{21}e^{-\eta_1^2/t} + 2e^{-(\eta_1+\eta_2)^2/t} + \ldots) \tag{21}$$

The calculation of the subsequent terms is increasingly cumbersome, but straightforward.

(21) immediately yields the asymptotic behaviour for $t \to 0$, (15) and (18). In particular, the plateau in $e(t)$ reaches up to a time of order η_1^2 (cf. Fig. 10 in [1]). The series (21) and its generalizations for more layers simplify when there are thick layers in the stack having large η values (see Eq. (9)).

One may now connect series (1) and (20), in order to solve the cut-off problem for them. This means that for $t \leqslant t_c$ one uses (20), and for $t > t_c$ (1). (This split-off resembles Ewald's method of calculating lattice sums [9].) When $\eta_2 \gg \eta_1$, one may choose $t_c = \eta_1^2$. If $t_c > t_{\min}$ in (19), the latter is weakened to

$$n_{\max} \gg \eta/\pi\sqrt{t_c} = \eta/\pi\eta_1 \tag{22}$$

For the example mentioned after (19), this brings a reduction of $n_{\max}$ by a factor of $\sqrt{20}$, which results in a considerable lowering of the computer time. Of course, in special cases, t_c may be chosen even more favourably.

3. *Numerical results and discussion*

We have tested the validity of the approximations proposed above by means of the three-layer model in [1]. The model parameters are listed in Table 1. For the short-time calculations $t \leqslant t_c$, we have expanded

$$\bar{\theta}(s) = \frac{1}{e_1\sqrt{s}} \cdot \frac{C_1(e_{12}S_2S_3 + e_{13}C_2C_3) + S_1(C_2S_3 + e_{23}S_2C_3)}{S_1(e_{12}S_2S_3 + e_{13}C_2C_3) + C_1(C_2S_3 + e_{23}S_2C_3)} \tag{23}$$

with $e_{ij} = e_i/e_j$, $S_i = sh(\eta_i\sqrt{s})$ and $C_i = ch(\eta_i\sqrt{s})$. (The corresponding series (1) is given by Eq. (26) in [1]). Due to $\eta_3^2 \gg \eta_3^2 \gg \eta_1^2$ (see Table 1), the series corresponding to (20) simplifies to

$$\Theta(t) = \frac{1}{e_1\sqrt{\pi t}}(1 + 2x_{41}e^{-\eta_1^2/t} + 2x_{41}^2 e^{-4\eta_1^2/t} + + 2x_{41}^3 e^{-9\eta_1^2/t} + 2x_{21}e^{-(\eta_1+\eta_2)^2/t}) \tag{24}$$

Table 1 Three-layer model in [1] (Table 1; Stolwijk and Hardy [10] model for living human skin)

Layer i	L_i, 10^{-4} m	$\varkappa_i$, 10^{-8} m^2 s^{-1}	e_i, kJ/m^{-2} s$^{-1/2}$ K^{-1}	η_i, s$^{1/2}$
1	1	4.9	.95	.452
2	7	9.7	1.34	2.25
3	100[a]	7.9	.60	35.5

[a] D. L. Balageas, priv. commun.

with $x_{41} = x_4/x_1 = -0.170$ and $x_{21} = x_2/x_1 = 0.381$. $t_c = 2\eta_1^2$ is chosen, which guarantees (24) as a good approximation.

Figure 1 displays our results for $e(t)$; the front-surface temperature history is less sensitive to the calculation details; we recovered Fig. 9 of [1]. We used 20 exact eigenvalues in (1) with a total of 250 terms at t_c (cf. Table 2). The step of $e(t)$ at t_c is actually less than 10 per cent (the logarithmic scale overdraws it somewhat).

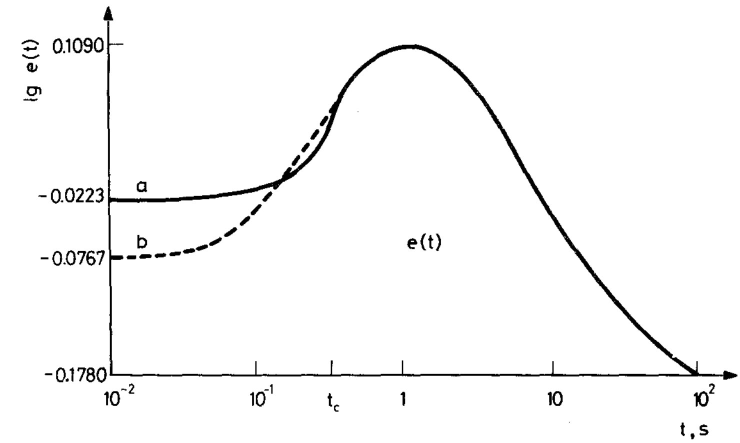

Fig. 1 History of the appearent effusivity, $e(t)$, after Dirac-pulse excitation of unit strength (cf. text). (a) series matching at $t_c = 2\eta_1^2 = 0.205$ s; (b) using only (1) with 250 terms

Table 2 Convergence of eigenvalues and prefactors in (1) towards their asymptotic values for the three-layer model in (1) (parameters given in Table 1)

n	$\gamma_n = \eta_3/\sqrt{\tau_n}$		F_n	
	exact	asympt.	exact	asympt.
14	41.172	40.881	1.4385	1.605
15	43.879	43.801	1.5679	1.5808
16	46.61	46.721	1.334	1.354
17	49.434	49.641	.9853	1.0483
18	52.348	52.561	.7197	.7737
19	55.323	55.481	.5567	.5772
20	58.334	58.401	.4659	.4648
100	292.11	292.005	—	—

In summary, satisfactory results can be obtained with small effort in comparison with the standard series. Moreover, the asymptotics of the decay constants enables one to perform (1) as a lattice sum, which lifts the matching problem. This will be described elsewhere.

Appendix A. Conversion of surface excitation into volume excitation

Surface excitation is usually incorporated in the boundary conditions (e.g. [1]). This may prevent the direct application of Fourier's method of separation of variables, for which it is more convenient to have the excitation term in the balance (diffusion) equation, where it may be called volume excitation. For this, and in order to prove that the asymptotics of eigenvalues is independent of the surface excitation too, we show how the inhomogeneity of the boundary condition can be removed by converting the surface excitation into a volume excitation. Consider for simplicity the problem

$$\frac{1}{\varkappa}\dot{\theta} = \theta'' + f(x, t) \tag{A. 1a}$$

$$-K\theta'(0, t) = b(t), \quad \theta'(L, t) = 0, \quad \theta(x, 0) = 0 \tag{A. 1b}$$

According to Duhamel's theorem [11], this is connected with the simpler one

$$\frac{1}{\varkappa}\dot{T} = T'' + f(x, u) \tag{A. 2a}$$

$$-KT'(0, t; u) = b(u), \quad T'(L, t; u) = 0, \quad T(x, 0; u) = 0 \tag{A. 2b}$$

by

$$\theta(x, t) = \frac{\partial}{\partial t}\int_0^t T(x, t-u; u)\,\mathrm{d}u \tag{A. 3}$$

Hence, it is sufficient to investigate the correspondence between $b(u)$ and $f(x, u)$ in (A. 2).

We solve (A. 2) by Laplace transformation and obtain

$$T(x, s; u) = Ae^{x\sqrt{s/\kappa}} + Be^{-x\sqrt{s/\kappa}} \tag{A. 4a}$$

with (i) for $f=0$:

$$\begin{aligned} A &= B - \varkappa^{1/2}b(u)/Ks^{3/2} \\ B &= \varkappa^{1/2}b(u)/(1-e^{-2L\sqrt{s/\kappa}})Ks^{3/2} \end{aligned} \tag{A. 4b}$$

and (ii) for $b=0$:

$$A = B + \frac{\varkappa^{1/2}}{s^{3/2}}\int_L^0 f(x, u)ch\left(x\sqrt{\frac{s}{\varkappa}}\right)\mathrm{d}x = Be^{-2L\sqrt{s/\kappa}} \tag{A. 4c}$$

Consequently, $b(t)$ in (A. 1b) can be replaced by $f(x, t) = \delta(x)b(t)/K$ in (A. 1a). This is the desired conversion.

Appendix B. Asymptotics of eigenvalues

Consider the eigenvalue equation for a two-layer system ([1], Eq. (22) with $R=0$),

$$x_1 \sin(\omega_1 \gamma) + x_2 \sin(\omega_2 \gamma) = 0 \tag{B. 1}$$

Writing

$$\gamma_n = \gamma_n^{as} + \delta_n/\omega_1 = n\pi/\omega_1 + \delta_n/\omega_1 \tag{B. 2}$$

we obtain

$$(-1)^n x_1 \sin \delta_n + x_2 \sin \frac{\omega_2}{\omega_1}(n\pi + \delta_n) = 0 \tag{B. 3}$$

$\delta_n = 0$ is a solution of (B. 3) only if $n\omega_2/\omega_1$ is an entire, but in general δ_n will be finite.

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Zusammenfassung — Es wurde gezeigt, daß bei quasi-eindimensionaler, linearer Fourier-Wärmeleitung in einer Packung von homogenen Schichten sich die Temperaturdämpfungskonstante τ_n asymptotisch als n^{-2} verhält. Dies ermöglicht bei Beibehaltung einer befriedigenden Genauigkeit eine erhebliche Einsparung von Computerzeit, wofür ein numerisches Beispiel angeführt wird. Es wurde das Anpassungsproblem für alternierende unendliche Reihen mit $e^{-t/\tau}$ bzw. $e^{-a/t}$ untersucht und die Äquivalenz von Oberflächen- und einigen Volumenanregungen dargestellt.

Резюме — В случае линейной, квазиодномерной теплопроводности пакетного набора гомогенных слоев было показано, что константы температурного затухания (τ_n) ведут себя как асимптомы n^{-2}. Это приводит к значительному понижению машинного времени при достаточном уровне точности. Приведен числовой пример. При этом учитывалась проблема согласования отборочных бесконечных рядов, содержащих термы $e^{-t/\tau}$ и $e^{-a/t}$ и показана равноценность между поверхностью и некотоьым объемным возбуждением.