Journal of Thermal Analysis, Vol. 34 (1988) 1301–1310

TRANSIENT HEAT CONDUCTION IN LAYERED MATERIALS: IMPROVED ASYMPTOTICS OF DECAY CONSTANTS

P. Enders

ZENTRALINSTITUT FÜR OPTIK UND SPEKTROSKOPIE DER AKADEMIE DER WISSENSCHAFTEN DER DDR.
RUDOWER CHAUSSEE 6, BERLIN 1199, G.D.R.

(Received October 12, 1987)

The asymptotic behaviour of the time constants in Fourier's series is given as $\tau_n \alpha \text{ const}/n^2$. Its utilization attempts to circumvent the transcendent eigenvalue equation for τ_n. This approximation can be substantially improved by means of Rayleigh's variational principle. A practical example demonstrates the usefulness of this approach, making practical calculations distinctly more effective.

Let us consider a linear transient Fourierean heat conduction problem in a stack of N homogeneous

$$\dot{\vartheta}(r, t) = \frac{1}{p} \nabla[\lambda \nabla \vartheta(r, t)] + Q(r, t) \tag{1}$$

separately for each layer ($\dot{(\,)} = \partial(\,)/\partial t$) and then matches these single-layer solutions according to the continuity of temperature, ϑ, and heat flux density, $-\lambda \nabla \vartheta$, across the interfaces (say, in the x-direction; λ and p are the heat conductivity and capacity, respectively, which are assumed to be constant within each layer). The compatibility requirement of these inner boundary conditions (BC) with the outer ones yields the eigenvalue equation, and thus the decay constants, τ_n, in Fourier's series

$$\vartheta(t) = \sum_n G_n e^{-t/\tau_n} \tag{2}$$

for the temperature history at some given point.

John Wiley & Sons, Limited, Chichester
Akadémiai Kiadó, Budapest

Obviously, the bottleneck of this method is the solution of the transcendental eigenvalue equation, the number of trigonometric summands of which grows roughly as 2^N.

In [3, 4] we have shown that this problem can be greatly simplified by utilizing the asymptotic behaviour

$$\tau_n \to (\eta/n\pi)^2 \quad \text{as} \quad n \to \infty \tag{3}$$

where

$$\eta = \sum_{i=1}^{N} \eta_i = \sum_{i=1}^{N} d_i/\varkappa_i^{1/2} \tag{4}$$

$\varkappa = \lambda/p$ (temperature conductivity or diffusivity), and d_i is the thickness of the i-th layer.

Here, we improve this asymptotics by means of Raleigh's variational principle [5] and extend the situation to multi-dimensional cases (heat spreading). After deriving this in section 2, in section 3 we consider a practical example and discuss the numerical results. Section 4 gives some conclusions. Finally, in the Appendix, we discuss the concept of apparent effusivity [7] for step excitation.

Variational principle

Within Fourier's method of separation of variables, one makes the ansatz

$$\vartheta(r, t) = T(t)X(x)Y(y)Z(z) \tag{5}$$

and gets

$$T(t) = T(0)e^{-t/\tau} \tag{6}$$

$$-\frac{1}{p(x)}[\lambda(x)X'(x)]' + \varkappa(x)\omega_{kl}^2 X(x) = \frac{1}{\tau}X(x) \tag{7}$$

($X' = \mathrm{d}X/\mathrm{d}x$, etc.), where $\omega_{kl}^2 = \mu_k^2 + \nu_l^2$, and

$$Y''(y) = -\mu_k^2 Y(y), \quad Z''(z) = -\nu_l^2 Z(z) \tag{8}$$

For adiabatic BC at the side walls:

$$\mu_k = 2k\pi/d_y, \quad \nu_l = 2l\pi/d_z \tag{9}$$

where $d_{y(z)}$ is the extension of the stack in the $y(z)$-direction.

It should be noted that (7) is not a Sturm–Liouville eigenvalue problem [6], since the coefficients jump at the interfaces. Nevertheless, one can perform a "partial" Sturm–Liouville transformation, which makes the coefficient of the second-derivation term constant. This leads to the asymptotics [3, 4].

Actually, the true τ_n-values oscillate around their asymptotic ones [3, 4] so we seek for an improvement of the latter.

If both sides of (7) are multiplied by $p(x)$, the differential operator on the l.h.s. becomes Hermitean [6], and we get

$$(\lambda X')' + \left(\frac{p}{\tau} - \lambda\omega_{kl}^2\right) X = 0 \tag{10}$$

The Gerjouy, Rau and Spruch [5] method of constructing variational principles (VP) then leads to the variational esimation [3]:

$$\left(\frac{1}{\tau}\right)_v = -||X_t||^{-2} \int_0^{d_x} X_t(\lambda X_t')' \, dx + \langle \tau_{kl}^{-1} \rangle \tag{11}$$

with

$$\begin{aligned} \tau_{kl}^{-1} &= \varkappa(x)\omega_{kl}^2, \quad ||X_t||^2 = \langle 1 \rangle, \\ \langle f(x) \rangle &= \int_0^{d_x} p(x) X_t^2(x) f(x) \, dx / \langle 1 \rangle \end{aligned} \tag{12}$$

This means that the deviation of $(\tau^{-1})_v$ from its true value is of the order ε^2 whenever the error in the trial function X_t with respect to the exact solution of (10) is of the order ε [5].

It is well known that the quality of a variational solution depends crucially on the proper choice of the trial function(s).

As in [3], we chose the asymptotic eigenfunctions corresponding to (3). The four combinations of outer BC of 1st and 2nd kind are listed in Table 1. For case 2

$$X_t = X_{nt}(x) = \cos \frac{1}{\sqrt{\tau_n}} \left(\bar{\eta}_i + \frac{x}{\sqrt{\varkappa_i}} \right), \quad 0 \leqslant x \leqslant d_i \tag{13}$$

$$\bar{\eta}_i = \sum_{j=1}^{i-1} \eta_j, \quad \bar{\eta}_1 = 0, \quad \bar{\eta}_2 = \eta_1, \quad \bar{\eta}_N = \eta - \eta_N. \tag{14}$$

Table 1 Asymptotic eigenvalues and eigenfunctions for the four harmonic BC; ξ is the argument in Eq. (13)

Case	$\eta/\pi\sqrt{\tau_n^{as}}$	X_n^{as}	BC
1	n	$\sin \xi/\sqrt{\tau_n}$	$X_n(0) = X_n(d_x) = 0$
2	$n-1/2$	$\cos \xi/\sqrt{\tau_n}$	$X_n'(0) = X_n(d_x) = 0$
3	$n-1/2$	$\sin \xi/\sqrt{\tau_n}$	$X_n(0) = X_n'(d_x) = 0$
4	n	$\cos \xi/\sqrt{\tau_n}$	$X_n'(0) = X_n'(d_x) = 0$

We then obtain

$$\langle \varkappa \rangle = \left(\frac{1}{2} \sum_{i=1}^{N} \lambda_i d_i + S_n^+ \right) \Big/ \langle 1 \rangle \tag{15}$$

and

$$\int_0^{d_x} (\lambda X'_{nt})' X_{nt} \, dx = -\tau_{nt}^{-1} \left(\frac{1}{2} \sum_{i=1}^{N} p_i d_i - S_n^- \right) \tag{17}$$

where

$$S_n^{\pm} = \frac{1}{4} \tau_{nt}^{1/2} \sum_{i=2}^{N} (\lambda_{i-1} \varkappa_{i-1}^{\pm 1/2} - \lambda_i \varkappa_i^{\pm 1/2}) \sin (2\bar{\eta}_i / \tau_{nt}^{1/2}) \tag{18}$$

Obviously, the sine factor in $S_n^{\pm}$ should produce oscillations of τ_n^{-1}. For instance, in the case of a quasi–1D two-layer stack, the first-order correction to (3) is [3]

$$\delta \frac{1}{\sqrt{\tau_n}} = \frac{e_2 - e_1}{\eta_1 e_1 + \eta_2 e_2} \sin \frac{2n\pi\eta_1}{\eta_1 + \eta_2}; \qquad e_i = (\lambda_i p_i)^{1/2} \tag{19}$$

Hence, up to the order ε^2, $\tau_n^{-1/2}$ oscillates as function of n with n-independent amplitude and frequency.

It now turns out that (3) is not an appropriate choice for τ_{nt} for multi-dimensional problems, since X_{nt} then contains no information about the lateral diffusion (heat spreading in the y- and/or z-direction) [3]. A better choice is

$$\tau_{nt}^{-1} = (n^* \pi / \eta)^2 + \langle \varkappa \rangle_0 \omega_{kl}^2, \quad n^* = n \text{ or } n - 1/2 \tag{20}$$

(cf. Table 1) (this influence of the outer BC on n^* was not considered in [4, 6]), for calculating $S_n^{\pm}$, where $\langle \varkappa \rangle_0$ can be calculated from (15) and (16) with the first term on the r.h.s. alone, i.e.

$$\langle \varkappa \rangle_0 = \sum_{i=1}^{N} \lambda_i d_i \Big/ \sum_{i=1}^{N} p_i d_i \tag{21}$$

τ_{nt} and X_{nt} can be further improved by successive repetition of this cycle (super-VP, cf. [5]).

Numerical results and discussion

Let us consider an 8-layer stack (stripe-laser chip), the parameters of which are listed in Table 2 [3]. We assume that layer 8 is mounted onto an ideal heat sink and that there is no heat loss on the side walls and on the upper surface. The power supply is provided by a current flow over the *pn* junction, assumed to be ideally thin and to lie at $x_0^{(3)} = 0.1$ μm in the middle of layer 3. The electric current is confined to a lateral width of $w_y = 6$ μm (but uniform in the z-direction), while the stack thickness is $d_y = 400$ μm. Since $w_y \ll d_y$, considerable heat spreading (excitation of many diffusion modes in the y-direction) is to be expected.

Table 2 Material constants of the 8-layer stack [3]

i	d_i, 10^{-6} m	$\varkappa_i$, 10^{-6} m^2 s^{-1}	λ_i, Wm^{-1} K^{-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

Thus, when the excitation is step-like, we have [3]

$$Q(r, t) = Q'_{s0} p_3^{-1} \delta(x_0^{(3)}) W(y) \theta(t) \tag{22}$$

$$W(y) = \theta(y + w_y/2) - \theta(y - w_y/2) \tag{23}$$

where $\theta(y)$ denotes Heaviside's step function and Q'_{s0} is the injected power per area.

The raising of the temperature at the *pn* junction, averaged over the lateral source width, w_y, is then described by

$$\vartheta_{pn}(t) = \sum_{k,n} G_{k,n} \tau_{n,k} (1 - \exp(-t/\tau_{n,k})) \tag{24}$$

The calculation of the prefactors is simple; one obtains [3]

$$G_{k,n} = Q'_{so} X_{n,k}^2 (x_0^{(3)}) \| X_{n,k} \|^{-2} \times \frac{2}{1 + \delta_{k0}} \frac{d_y}{w_y} \frac{1}{k^2 \pi^2} \sin^2 \left(k\pi \frac{w_y}{d_y} \right) \tag{25}$$

Here, $X_{n,k}$ are the solutions of (7) with $l = 0$.

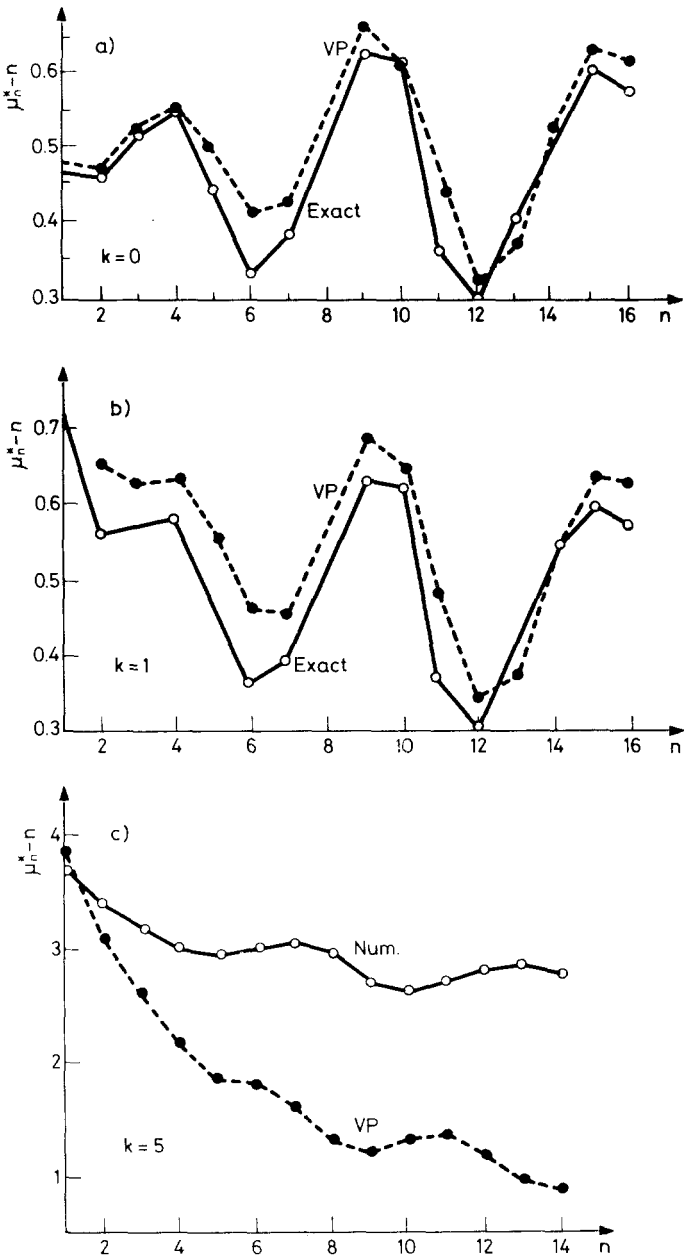

Fig. 1 Asymptotic behaviour of eigenvalues, $\mu_n = \tau_n^{-1/2}$; $\mu_n^* = \mu_n \eta/\pi$; a) $k=0$, b) $k=1$, c) $k=5$

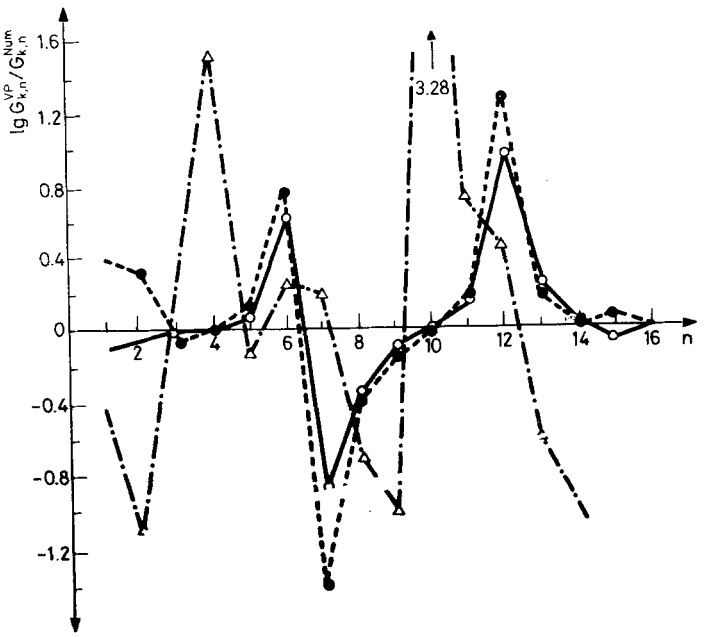

Fig. 2 Relative error of the approximative prefactors, $G_{k,n}^{VP}$, with respect to the numerically calculated values, $G_{k,n}^{num}$, for different k-values ($k = 0, 1, 5$)

Figure 1 displays the absolute error of the normalized eigenvalues (see Table 1, case 2). Clearly, a substantial improvement over (3) is gained by the simple VP approach outlined above. Naturally, the deviations grow with increasing k, since the trial values and functions are not very good for larger k.

Figure 2 shows the corresponding relative errors of the prefactor. The overall agreement is satisfactory; large errors are connected with very small values of one of the parameters. Within the total sum (24), however, they play a minor role.

The latter is demonstrated in Fig. 3, where $\vartheta_{pn}(t)$ and $e(t)$, the corresponding apparent effusivity (see Appendix), are drawn. At large times, $t \gtrsim \tau_{1,0}$, the accuracy of $\vartheta(t)$ depends mainly on that of $\tau_{1,0}$; for this, the largest differences in Fig. 3 occur at the end of the time scale. (The infinite series (24) was approximated by ~ 400 terms, 16 x- and 25 y-modes, including all time constants up to 0.2 μs. This approximation gives only 0.0580 K for the stationary value, $\vartheta_{pn}(\infty)$, while the exact one is 0.1296 K at $Q'_{s0} = 10^6$ Wm^{-2} [3]).

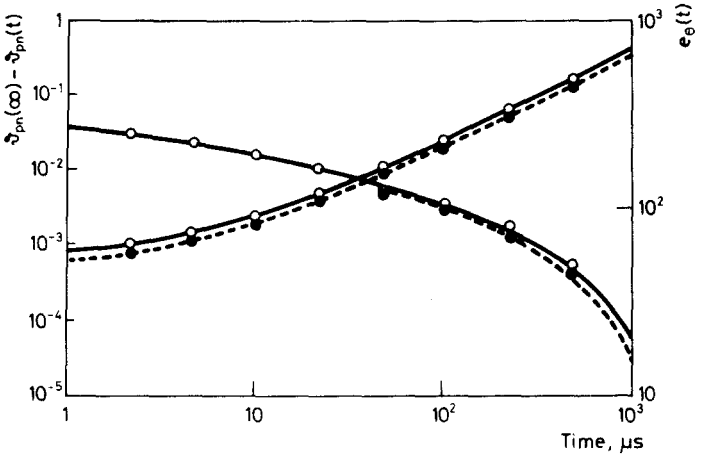

Fig. 3 Temperature and effusivity history at the *pn* junction calculated with the numerical (straight line) and with the asymptotic decay constants (broken line)

Conclusions

The calculation of the coefficients of Fourier's series (2) without solving the transcendent eigenvalue equation is a very appealing task, since it saves a large amount of computer time (see also [3, 8]). On the other hand, a priori, a knowledge of the asymptotic behaviour of the eigenvalues (time constants) helps effectively in searching for their exact values, since it yields their density. More precisely, $\eta/\pi\sqrt{\tau_n}$ has as function of n the mean density unit (cf. (3)), i.e. there is, on average, just one value between two adjacent integers (cf. Fig. 1).

The application of Rayleigh's VP (11) results in a significant improvement in the description of the asymptotic behaviour of the decay constants relative to (20) (see Fig. 1). Further improvement is possible with the super-VP [5], but the expense increases rapidly. As Fig. 3 shows, even the first correction can give quite satisfactory results.

To summarize, this approach may make practical calculations distinctly more effective.

Appendix. Apparent effusivity for step-like excitation

In the method of pulsed photothermal modelling of materials [7, 9], one defines an apparent effusivity

$$e_\delta(t) = Q_{s0}/\vartheta_\delta(t)\sqrt{\pi t} \tag{A.1}$$

where $\vartheta_\delta(t)$ is the front surface temperature after Dirac-pulse excitation. The effusivity as material parameter is defined as $e = (\lambda p)^{1/2}$; it is also called the heat penetration number ([2], p. 69). When the sample is thermally isolated after excitation, $e_\delta(t)$ evolved from $e_\delta(0) = e_1$, the effusivity of the excited layer, to $e_\delta(\infty) = 0$ (cf. [7]).

The advantage of plotting $e(t)$ is that it displays a much more pronounced structure than $\vartheta(t)$ [3, 7]. This structure corresponds to the penetration of heat through the layers, but not in one-to-one manner: the plateau of $e(t)$ near $t=0$ reaches up to about $\eta^2_{\min}$, independently of the position of the layer to which $\eta_{\min}$ belongs [4, 3].

In contrast, this behaviour near $t=0$ is completely changed, when the excitation is step-like (cf. (24)). Our aim is to modify (A.1) so as to obtain an $e_\theta(t)$ with similar behaviour as $e_\delta(t)$ obeys, especially near $t=0$ (plateau).

Due to the relation between the excitation shapes, we have $\vartheta_\delta(t) = \text{const} \cdot \mathrm{d}\vartheta_\theta(t)/\mathrm{d}t$. Furthermore, the plateau of $e_\delta(t)$ near $t=0$ is connected with the asymptotic behaviour

$$\vartheta_\delta(t) \to Q_{s0}/e_1 \sqrt{\pi t} \quad \text{as} \quad t \to 0 \tag{A.2}$$

(cf. (A.1)). From this it follows that

$$\vartheta_\theta(t) \to 2Q'_{s0} \sqrt{t}/e_1 \sqrt{\pi} \quad \text{as} \quad t \to 0 \tag{A.3}$$

Therefore, it seems reasonable to define

$$e_\theta(t) = 2Q'_{s0} \sqrt{t}/\vartheta_\theta(t) \sqrt{\pi} \tag{A.4}$$

When the sample does not lose heat, $\vartheta_\theta(t)$ will increase nearly linearly with $\sqrt{t}$, so that $e_\theta(t)$ evolves like $e_\delta(t)$, as invoked. In contrast, when there is a heat sink, a stationary temperature distribution develops, and $e_\theta(t)$ diverges as $t^{1/2}$ for $t \to \infty$. However, in this case, $e_\delta(t)$ diverges too, because $\vartheta_\delta(t)$ will fall exponentially ($\tau_0^{-1/2}$ is no longer an eigenvalue; cf. [3]).

Figure 3 gives an example for the latter case.

References

1 H. S. Carslaw and J. C. Jaeger, Conduction of Heat in Solids, 2nd ed., Oxford U.P., London 1959.

2 H. Tautz, Wärmeleitung und Temperaturausgleich, Akademie-Verlag, Berlin 1971.

3 J. Galley and P. Enders, Heat Transfer in Multilayer Systems. Limits of "Classical" Diffusion Theory, ZOS-Prepring 87–7, Berlin 1987.

4 P. Enders, J. Thermal Anal., 34 (1988) 319.

5 E. Gerjuoy, A. R. P. Spruch and L. Spruch, Rev. Mod. Phys., 55 (1983) 725.

6 H. J. Dirschmidt, W. Kummer and M. Schweda, Einführung in die mathematischen Methoden der Theoretischen Physik, Vieweg, Braunschweig 1976, Ch. 4.
7 D. L. Balageas, J. C. Krapez and P. Cielo, J. Appl. Phys., 59 (1986) 348.
8 P. Enders, J. Thermal Anal., 34 (1988) 871.
9 P. Cielo, J. Appl. Phys., 56 (1984) 230.

Zusammenfassung — Das asymptotische Verhalten der Zeitkonstanten in Fouriers Reihe ist $\tau_n \alpha \text{ const}/n^2$. Sein Gebrauch zielt auf die Umgehung der transzendenten Eigenwertgleichung für τ_n. Diese Näherung kann mit Hilfe des Rayleighschen Variationsprinzips wesentlich verbessert werden. Ein praktisches Beispiel zeigt die Nützlichkeit dieses Zuganges, der eine deutliche Effektivierung praktischer Rechnungen liefert.

Резюме — Азимптотическое поведение временных постоянных в рядах фурьера есть $\tau_n \alpha \text{ const}/n^2$. Его употребление направлено на избежание трансцендентного уравнения для τ_n. Это приближение может быть существенно улучшенным посредством вариационного принципа Релея. Практический пример показывает ценность этого подхода, приводящего к значительному повышению эффективности практических расчетов.