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Heat Diffusion 3D model

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1 Motivation

The aim is to obtain the analytical expression of the continuous component of the laser-induced temperature rise in a layer on a substrate in good thermal contact with a thermostat and in a layer in bad thermal contact with a thermostat (contact thermal resistance). The results were given in the following paper without detailed calculation:

JOURNAL OF APPLIED PHYSICS 119, 153904 (2016)

Steady-state thermal gradient induced by pulsed laser excitation in a ferromagnetic layer

S. Shihab, 1 L. Thevenard, 1 A. Lemaitre, 2 J.-Y. Duquesne, 1 and C. Gourdon 1

In the case of a layer on a substrate in good thermal contact with a thermostat, the temperature rise at the surface is given by Eq. 1, which reads:
2 TWO-LAYER SAMPLE IN CONTACT WITH A THERMOSTAT

\[
\Delta T(r) = \frac{P_0(1 - \Re)}{2\pi} \int_0^\infty f(u) e^{-\frac{u^2}{2\sigma^2}} J_0(ru) du
\]

\[
f(u) = \frac{k_1 \cosh(uL_1) \sinh(uL_0) + k_0 \sinh(uL_1) \cosh(uL_0)}{k_1(k_1 \sinh(uL_1) \sinh(uL_0) + k_0 \cosh(uL_1) \cosh(uL_0))^{\frac{1}{2}}}
\]

and in the case of a single layer in bad thermal contact with a thermostat, the temperature rise is given by Eq. 2, which reads:

\[
\Delta T(r, z) = \frac{P_0(1 - \Re)}{2\pi} \int_0^\infty g(u, z) e^{-\frac{u^2}{2\sigma^2}} J_0(ru) du,
\]

\[
g(u, z) = \frac{a}{k(u^2 - \sigma^2)} \times \left( \frac{\cosh(uz)(ze^{-Lu}(1 - kRu) + ue^{-\sigma z}(zkR - 1))}{kRu \sinh(Lu) + \cosh(Lu)} \right.
\]

\[
\left. + ue^{-\sigma z} - ze^{-uz} \right)
\]

2 Two-layer sample in contact with a thermostat

The heat diffusion equation is written as

\[
\frac{\partial \Delta T}{\partial t} - D \nabla^2 \Delta T = p(r, z, t) / \rho C,
\]

with $\Delta T = T - T_{\text{thermostat}}$, $D$ the diffusivity, $p$ the absorbed power per unit volume, $\rho$ the mass density and $C$ the mass specific heat. $T_{\text{thermostat}}$ is the base temperature. The continuous component of $\Delta T$ is found as the solution
of the time-independent diffusion equation in response to the time-averaged absorbed power (CW component).

Here the system under consideration is a layer of thickness $L_1$ and thermal conductivity $k_1$ on top of a substrate of thickness $L_0$ and thermal conductivity $k_0$ in contact with a thermostat (Fig. 2.1).

![Figure 2.1:](image)

We first assume that the energy flux from the laser transmitted at the surface ($z=0$) is totally converted into heat flux within an infinitely thin depth.

The temperature and the heat flux at the layer/substrate interface are continuous functions of the depth $z$ in the case of zero contact resistance at each interface. The sample is perfectly thermalized at the substrate-thermostat interface, i.e., $\Delta T = T(r, L_0 + L_1) - T_{thermostat} = 0$.

In the continuous regime and without volume heat source the heat diffusion equation in each layer is reduced to:

$$\nabla^2 \Delta T = 0 \quad (2.2)$$

which in cylindrical coordinates translates to

$$\frac{\partial^2 \Delta T}{\partial r^2} + \frac{1}{r} \frac{\partial \Delta T}{\partial r} + \frac{\partial^2 \Delta T}{\partial z^2} = 0 \quad (2.3)$$

$\Delta T(r, z)$ is written as a function of its Hankel transform $\Theta(r, z)$ as $\Delta T(r, z) = \int_0^{+\infty} \Theta(u, z) J_0(ru) u \, du$, where $J_0$ is the Bessel Function of the first kind. The Hankel transform then verifies
\[ \frac{\partial^2 \Delta T}{\partial r^2} + \frac{1}{r} \frac{\partial \Delta T}{\partial r} + \frac{\partial^2 \Delta T}{\partial z^2} = \int_0^{+\infty} \left( -u^2 \Theta(u, z) + \frac{\partial^2 \Theta(u, z)}{\partial z^2} \right) J_0(r u) \, u \, du \] (2.4)

The solutions of \( -u^2 \Theta(u, z) + \frac{\partial^2 \Theta(u, z)}{\partial z^2} \) = 0 are then

\[ \Theta(u, z) = A_{1,0}(u) \exp(-u z) + B_{1,0}(u) \exp(u z), \] (2.5)

Where the two indices 1 and 0 refer to the layer and the substrate, respectively. The functions \( A \) and \( B \) are determined by the boundary conditions.

At the surface, the incoming heat flux \( \phi(r) \), which has cylindrical symmetry is equal to the normal flux at \( z=0 \).

\[ -k_1 \frac{\partial \Delta T}{\partial z} = \phi(r) \] (2.6)

Taking the Hankel transform on both side, we have (condition 1)

\[ -k_1 \frac{\partial \Theta}{\partial z} = \psi(u) \] (2.7)

with \( \psi(u) = \int_0^{+\infty} \phi(u, z) J_0(r u) \, r \, dr \), the Hankel transform of \( \phi \).

Condition 2 and 3 are given by the continuity of the temperature and the heat flux at the layer-substrate interface. Condition 4 is given by the continuity of the temperature at the substrate-thermostat interface \( \Delta T(r, L_0 + L_1) = 0 \). The four conditions then lead to the following set of equations:

\[ k_1 u (A_1(u) - B_1(u)) = \psi(u) \] (2.8)

\[ A_1(u) \exp(-u L_1) + B_1(u) \exp(u L_1) = A_0(u) \exp(-u L_1) + B_0(u) \exp(u L_1) \] (2.9)

\[ k_0 u [A_1(u) \exp(-u L_1) - B_1(u) \exp(u L_1)] = k_0 u [A_0(u) \exp(-u L_1) - B_0(u) \exp(u L_1)] \] (2.10)

\[ A_0(u) \exp(-u (L_0 + L_1)) + B_0(u) \exp(u (L_0 + L_1)) = 0 \] (2.11)
Solving this system gives the functions $A_1(u)$ and $B_1(u)$:

\[
A_1(u) = \psi(u) \frac{e^{L_1u} [k_1 \sinh (L_0u) + k_0 \cosh (L_0u)]}{2k_1u [k_1 \sinh (L_0u) \sinh (L_1u) + k_0 \cosh (L_0u) \cosh (L_1u)]}
\]

(2.12)

\[
B_1(u) = \psi(u) \frac{e^{-L_1u} [k_1 \sinh (L_0u) - k_0 \cosh (L_0u)]}{2k_1u [k_1 \sinh (L_0u) \sinh (L_1u) + k_0 \cosh (L_0u) \cosh (L_1u)]}
\]

(2.13)

The temperature at the surface ($z = 0$) is expressed as

\[
\Delta T(r, 0) = \int_0^{+\infty} (A_1(u) + B_1(u)) J_0(ru) \, du
\]

(2.14)

Since the laser spot is well fitted by a Gaussian, the incident flux is taken as $\phi(r) = \phi_0 \exp\left(-\frac{2r^2}{w^2}\right)$. The measured incident power is:

\[
P_0 = \int_0^{+\infty} \phi_0 \exp\left(-\frac{2r^2}{w^2}\right) 2\pi r \, dr = \frac{\pi w^2 \phi_0}{2}.
\]

(2.15)

The incoming flux has to be corrected by a factor $(1 - R)$, where $R$ is the reflectance. Therefore the incoming flux is expressed as $\frac{2P_0(1-R)}{\pi w^2} \exp\left(-\frac{2r^2}{w^2}\right)$

and its Hankel transform $\psi(u) = \int_0^{+\infty} \left(\frac{2P_0(1-R)}{\pi w^2} \exp\left(-\frac{2r^2}{w^2}\right)\right) J_0(ru) \, r \, dr$ is equal to $\frac{P_0(1-R)}{2\pi} \exp\left(-\frac{1}{8}u^2w^2\right)$.

Finally, combining Eqs 2.12, 2.13 with the expression of $\psi(u)$, one obtains:

\[
\Delta T(r, 0) = \frac{P_0(1-R)}{2\pi} \int_0^{+\infty} \exp\left(-\frac{1}{8}u^2w^2\right) f(u) \, J_0(ru) \, du,
\]

(2.16)

with

\[
f(u) = \frac{k_0 \sinh (L_1u) \cosh (L_0u) + k_1 \sinh (L_0u) \cosh (L_1u)}{k_1 (k_1 \sinh (L_0u) \sinh (L_1u) + k_0 \cosh (L_0u) \cosh (L_1u))},
\]

(2.17)

which is actually Eq. 1 of the paper quoted above.
3 Single layer and contact thermal resistance at the layer-thermostat interface

The system is now a single layer with thickness $L$ and thermal conductivity $k$ (Fig. 3.1). We assume that it is in bad thermal contact with a thermostat, i.e., there is a temperature discontinuity at the layer-substrate interface owing to a contact thermal resistance.

![Diagram of a single layer and thermostat](image)

Figure 3.1: Now we explicitly take into account the light absorption depth. We solve the heat diffusion equation $-D \nabla^2 \Delta T = p(r,z)/\rho C$, which is also written as $\nabla^2 \Delta T = -p(r,z)/k$. Taking the radial and depth dependence of absorbed power per unit volume as $p(r,z) = p_0 \exp\left(-\frac{2r^2}{w^2}\right) \exp\left(-\alpha z\right)$, we have $P_0(1-R) = \int_0^{+\infty} p_0 \exp\left(-\frac{2r^2}{w^2}\right) \exp\left(-\alpha z\right) 2\pi r \, dr \, dz$, therefore $p_0 = \frac{2\alpha P_0(1-R)}{\pi w^2}$. We have now to solve the following equation:

$$
\frac{\partial^2 \Delta T}{\partial r^2} + \frac{1}{r} \frac{\partial \Delta T}{\partial r} + \frac{\partial^2 \Delta T}{\partial z^2} = \int_0^{+\infty} \left(-u^2 \Theta(u,z) + \frac{\partial^2 \Theta(u,z)}{\partial z^2}\right) J_0(ru) \, u \, du
$$

$$
= \frac{1}{k} \int_0^{\infty} \Pi(u) J_0(ru) \, u \, du ,
$$

where $\Pi(u,z)$ is the Hankel transform of $p(r,z)$, i.e.,

$$
\Pi(u,z) = \frac{\alpha P_0(1-R)}{2\pi} \exp\left(-\frac{1}{8} u^2 w^2\right) \exp\left(-\alpha z\right) \quad (3.1)
$$

$$
= \Pi_0 \exp\left(-\frac{1}{8} u^2 w^2\right) \exp\left(-\alpha z\right)
$$
3 SINGLE LAYER AND CONTACT THERMAL RESISTANCE AT
THE LAYER- THERMOSTAT INTERFACE

with \( \Pi_0 = \frac{\alpha \Pi_0 (1 - R)}{2\pi} \). The solutions are found by solving

\[
-u^2 \Theta(u, z) + \frac{\partial^2 \Theta(u, z)}{\partial z^2} = -\frac{1}{k} \Pi(u, z)
\]

(3.2)

We then have

\[
\Theta(u, z) = A(u) \exp(-uz) + B(u) \exp(uz) + \frac{\Pi_0}{k(u^2 - \alpha^2)} \exp\left(-\frac{1}{8} u^2 w^2\right) \exp(-\alpha z)
\]

(3.3)

The functions \( A \) and \( B \) are found by solving the boundary conditions using the Hankel transform. The flux across the interface at \( z=0 \) is zero \((-k \frac{\partial \Theta}{\partial z} = 0)\), which gives:

\[
u (-A(u) + B(u)) - \frac{\alpha \Pi_0}{k(u^2 - \alpha^2)} \exp\left(-\frac{1}{8} u^2 w^2\right) = 0
\]

(3.4)

At the layer-thermostat interface there is a temperature discontinuity owing to the contact thermal resistance \( R_c \). We thus have:

\[
T(r, z = L^+) - T(r, z = L^-) = -R_c \left(-k \frac{\partial T}{\partial z} \bigg|_{z=L}\right)
\]

\[
\Delta T(r, L^-) = R_c \left(-k \frac{\partial \Delta T}{\partial z} \bigg|_{z=L}\right)
\]

\[
\Theta(u, L^-) = - R_c k \frac{\partial \Theta}{\partial z} \bigg|_{z=L}
\]

\[
A \exp(-uL) + B \exp(uL) + \frac{\Pi_0}{k(u^2 - \alpha^2)} \exp\left(-\frac{1}{8} u^2 w^2\right) \exp(-\alpha L) +
\]

\[R_c k \left(-Au \exp(-uL) + Bu \exp(uL) - \frac{\alpha \Pi_0}{k(u^2 - \alpha^2)} \exp\left(-\frac{1}{8} u^2 w^2\right) \exp(-\alpha L)\right) = 0
\]

(3.5)
From Eqs 3.4 and 3.5, one finds for \( A(u) \) and \( B(u) \) :

\[
A(u) = -\frac{e^{ Lu}(\alpha e^{ Lu}(kR_cu + 1) + ue^{-\alpha L}(1 - \alpha kR_c))}{ku (u^2 - \alpha^2)(e^{2Lu}(kR_cu + 1) - kR_cu + 1)} \Pi_0 \exp \left( -\frac{u^2 w^2}{8} \right)
\]

\[
B(u) = \frac{e^{-\alpha L}(\alpha e^{\alpha L}(1 - kR_cu) - ue^{ Lu}(1 - \alpha kR_c))}{ku (u^2 - \alpha^2)(e^{2Lu}(kR_cu + 1) - kR_cu + 1)} \Pi_0 \exp \left( -\frac{u^2 w^2}{8} \right)
\]

The radial and z-dependence of the temperature are then obtained as:

\[
\Delta T(r, z) = \int_0^{+\infty} \left( A(u) \exp(-uz) + B(u) \exp(uz) \right) J_0 \left( ru \right) u du + \frac{\Pi_0}{k(u^2 - \alpha^2)} \exp \left( -\frac{1}{8} u^2 w^2 \right) \exp(-\alpha z) J_0 \left( ru \right) u du
\]

which, after some algebra, gives Eq. 2 of the above paper, namely:

\[
\Delta T(r, z) = \frac{P_0 (1 - R)}{2\pi} \int_0^{\infty} g(u, z) \exp \left( -\frac{u^2 w^2}{8} \right) J_0 \left( ru \right) du,
\]

with \( g(u, z) = \frac{\alpha}{k(u^2 - \alpha^2)} \left( \frac{\cosh(uz)\left( \alpha e^{-Lu}(1 - kR_cu) + \alpha e^{-Lu}(\alpha kR_c - 1) \right)}{kR_cu \sinh(Lu) + \cosh(Lu)} + \alpha e^{-uz} \right). \)