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:

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

S. Shihab,[1] L. Thevenard,[1] A. Lemaître,[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:

$$\Delta T(r) = \frac{P_0(1-\Re)}{2\pi}\int_0^\infty f(u) e^{-\frac{1}{8}u^2w^2} J_0(ru)\,du$$
$$f(u) = \frac{k_1\cosh(uL_1)\sinh(uL_0) + k_0\sinh(uL_1)\cosh(uL_0)}{k_1\left(k_1\sinh(uL_1)\sinh(uL_0) + k_0\cosh(uL_1)\cosh(uL_0)\right)}, \quad (1)$$

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:

$$\Delta T(r,z) = \frac{P_0(1-\Re)}{2\pi}\int_0^\infty g(u,z) e^{-\frac{1}{8}u^2w^2} J_0(ru)\,du,$$
$$g(u,z) = \frac{\alpha}{k(u^2-\alpha^2)} \times \left(\frac{\cosh(uz)(\alpha e^{-Lu}(1-kRu) + ue^{-\alpha L}(\alpha kR - 1))}{kRu\sinh(Lu) + \cosh(Lu)} + ue^{-\alpha z} - \alpha e^{-uz}\right). \quad (2)$$

2 Two-layer sample in contact with a thermostat

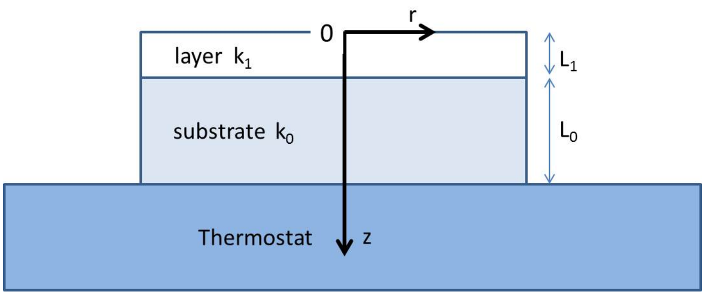
The heat diffusion equation is written as

$$\partial\Delta T/\partial t - D\nabla^2\Delta T = p\,(r,z,t)\,/\rho C, \quad (2.1)$$

with $\Delta T = T - T_{thermostat}$, D the diffusivity, p the absorbed power per unit volume, ρ the mass density and C the mass specific heat. $T_{thermostat}$ is the base temperature. The continuous component of ΔT 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:



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., $\Delta T = T\left(r, L_0 + L_1\right) - T_{thermostat} = 0$.

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

$$\nabla^2 \Delta T = 0 \tag{2.2}$$

which in cylindrical coordinates translates to

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

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

$$\frac{\partial^2 \Delta T}{\partial r^2} + \frac{1}{r}\frac{\partial \Delta T}{\partial r} + \frac{\partial^2 \Delta T}{\partial z^2} = \int_0^{+\infty} \left(-u^2 \Theta(u,z) + \frac{\partial^2 \Theta(u,z)}{\partial z^2} \right) J_0\,(ru)\, u\, du \tag{2.4}$$

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

$$\Theta(u,z) = A_{1,0}\,(u) \exp\,(-uz) + B_{1,0}\,(u) \exp\,(uz)\ , \tag{2.5}$$

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.

$$-k_1 \frac{\partial \Delta T}{\partial z} = \phi\,(r) \tag{2.6}$$

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

$$-k_1 \frac{\partial \Theta}{\partial z} = \psi\,(u) \tag{2.7}$$

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

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:

$$k_1 u\,(A_1\,(u) - B_1\,(u)) = \psi\,(u) \tag{2.8}$$

$$\begin{aligned} A_1\,(u) \exp\,(-u\,L_1) + B_1\,(u) \exp\,(u\,L_1) &= \\ A_0\,(u) \exp\,(-u\,L_1) + B_0\,(u) \exp\,(u\,L_1) & \end{aligned} \tag{2.9}$$

$$\begin{aligned} k_1 u\,[A_1\,(u) \exp\,(-u\,L_1) - B_1\,(u) \exp\,(u\,L_1)] &= \\ k_0 u\,[A_0\,(u) \exp\,(-u\,L_1) - B_0\,(u) \exp\,(u\,L_1)] & \end{aligned} \tag{2.10}$$

$$A_0\,(u) \exp\,(-u\,(L_0 + L_1)) + B_0\,(u) \exp\,(u\,(L_0 + L_1)) = 0 \tag{2.11}$$

Solving this system gives the functions $A_1(u)$ and $B_1(u)$:

$$A_1(u) = \psi(u)\frac{e^{L_1 u}\left[k_1 \sinh(L_0 u) + k_0 \cosh(L_0 u)\right]}{2k_1 u\left[k_1 \sinh(L_0 u)\sinh(L_1 u) + k_0 \cosh(L_0 u)\cosh(L_1 u)\right]} \tag{2.12}$$

$$B_1(u) = \psi(u)\frac{e^{-L_1 u}\left[k_1 \sinh(L_0 u) - k_0 \cosh(L_0 u)\right]}{2k_1 u\left[k_1 \sinh(L_0 u)\sinh(L_1 u) + k_0 \cosh(L_0 u)\cosh(L_1 u)\right]} \tag{2.13}$$

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

$$\Delta T(r, 0) = \int_0^{+\infty} \left(A_1(u) + B_1(u)\right) J_0(ru)\, u\, du \tag{2.14}$$

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:

$$P_0 = \int_0^{+\infty} \phi_0 \exp\left(-\frac{2r^2}{w^2}\right) 2\pi r\, dr = \frac{\pi w^2 \phi_0}{2}. \tag{2.15}$$

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 $\frac{P_0(1-R)}{2\pi} \exp\left(-\frac{1}{8}u^2 w^2\right)$.
Finally, combining Eqs 2.12, 2.13 with the expression of $\psi(u)$, one obtains:

$$\Delta T(r, 0) = \frac{P_0(1-R)}{2\pi} \int_0^{+\infty} \exp\left(-\frac{1}{8}u^2 w^2\right) f(u)\, J_0(ru)\, du\ , \tag{2.16}$$

with

$$f(u) = \frac{k_0 \sinh(L_1 u)\cosh(L_0 u) + k_1 \sinh(L_0 u)\cosh(L_1 u)}{k_1\left(k_1 \sinh(L_0 u)\sinh(L_1 u) + k_0 \cosh(L_0 u)\cosh(L_1 u)\right)}\ , \tag{2.17}$$

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.

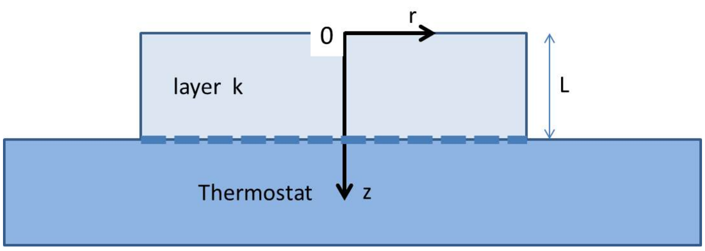


Figure 3.1:

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

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

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

$$\Pi\left(u,z\right) = \frac{\alpha P_0(1-R)}{2\pi}\exp\left(-\frac{1}{8}u^2w^2\right)\exp\left(-\alpha\, z\right) \tag{3.1}$$
$$= \Pi_0\exp\left(-\frac{1}{8}u^2w^2\right)\exp\left(-\alpha\, z\right)$$

with $\Pi_0 = \frac{\alpha P_0(1-R)}{2\pi}$. The solutions are found by solving

$$-u^2\Theta(u,z) + \frac{\partial^2\Theta(u,z)}{\partial z^2} = -\frac{1}{k}\Pi\left(u,z\right) \tag{3.2}$$

We then have

$$\Theta(u,z) = A\left(u\right)\exp\left(-uz\right)+B\left(u\right)\exp\left(uz\right)+\frac{\Pi_0}{k\left(u^2-\alpha^2\right)}\exp\left(-\frac{1}{8}u^2w^2\right)\exp\left(-\alpha\, z\right) \tag{3.3}$$

The functions A and$B$ are found by solving the boundary conditions using the Hankel transform. The flux accross the interface at z=0 is zero $\left(-k_1\frac{\partial\Theta}{\partial z}=0\right)$, which gives:

$$u\left(-A\left(u\right)+B\left(u\right)\right) - \frac{\alpha\,\Pi_0}{k\left(u^2-\alpha^2\right)}\exp\left(-\frac{1}{8}u^2w^2\right) = 0 \tag{3.4}$$

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

$$\begin{aligned} T\left(r,z=L^+\right)-T\left(r,z=L^-\right) &= -R_c\left(-k\left.\frac{\partial T}{\partial z}\right|_{z=L}\right) \\ \Delta T\left(r,L^-\right) &= R_c\left(-k\left.\frac{\partial \Delta T}{\partial z}\right|_{z=L}\right) \\ \Theta(u,L^-) &= -\ R_c\,k\left.\frac{\partial\Theta}{\partial z}\right|_{z=L} \end{aligned}$$

$$\begin{aligned} A\exp\left(-uL\right)+B\exp\left(uL\right)+\frac{\Pi_0}{k\left(u^2-\alpha^2\right)}\exp\left(-\frac{1}{8}u^2w^2\right)\exp\left(-\alpha\,L\right) \quad + \\ R_c\,k\left(-Au\,\exp\left(-uL\right)+Bu\,\exp\left(uL\right)-\frac{\alpha\Pi_0}{k\left(u^2-\alpha^2\right)}\exp\left(-\frac{1}{8}u^2w^2\right)\exp\left(-\alpha\,L\right)\right) \quad = \quad 0 \end{aligned} \tag{3.5}$$

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

$$A(u) = -\frac{e^{Lu}\left(\alpha e^{Lu}(kR_c u+1)+ue^{-\alpha L}(1-\alpha kR_c)\right)}{ku\left(u^2-\alpha^2\right)\left(e^{2Lu}(kR_c u+1)-kR_c u+1\right)}\Pi_0 \exp\left(-\frac{u^2w^2}{8}\right) \quad (3.6)$$

$$B(u) = \frac{e^{-\alpha L}\left(\alpha e^{\alpha L}(1-kR_c u)-ue^{Lu}(1-\alpha kR_c)\right)}{ku\left(u^2-\alpha^2\right)\left(e^{2Lu}(kR_c u+1)-kR_c u+1\right)}\Pi_0 \exp\left(-\frac{u^2w^2}{8}\right) \quad (3.7)$$

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

$$\Delta T(r,z) = \int_0^{+\infty}\Bigg(A(u)\exp(-uz)+B(u)\exp(uz) + \frac{\Pi_0}{k\left(u^2-\alpha^2\right)}\exp\left(-\frac{1}{8}u^2w^2\right)\exp(-\alpha\, z)\Bigg) J_0(ru)\,u\,du \quad (3.8)$$

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

$$\Delta T(r,z) = \frac{P_0(1-R)}{2\pi}\int_0^{\infty} g(u,z)\exp\left(-\frac{u^2w^2}{8}\right) J_0(ru)\; du\;, \quad (3.9)$$

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