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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

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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:

$$\Delta T(r) = \frac{P_0(1-\Re)}{2\pi} \int_0^\infty f(u) e^{-\frac{1}{8}u^2 w^2} J_0(ru) \, du$$

$$f(u) = \frac{k_1 \cosh(uL_1) \sinh(uL_0) + k_0 \sinh(uL_1) \cosh(uL_0)}{k_1 \left(k_1 \sinh(uL_1) \sinh(uL_0) + k_0 \cosh(uL_1) \cosh(uL_0)\right)},$$
(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:

$$\Delta T(r,z) = \frac{P_0(1-\Re)}{2\pi} \int_0^\infty g(u,z) e^{-\frac{1}{8}u^2 w^2} J_0(ru) \, du,$$

$$g(u,z) = \frac{\alpha}{k(u^2 - \alpha^2)}$$

$$\times \left(\frac{\cosh(uz)(\alpha e^{-Lu}(1-kRu) + ue^{-\alpha L}(\alpha kR - 1))}{kRu\sinh(Lu) + \cosh(Lu)} + ue^{-\alpha z} - \alpha e^{-uz} \right).$$
(2)

2 Two-layer sample in contact with a thermostat

The heat diffusion equation is written as

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

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).



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 :

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

which in cylindrical coordinates translates to

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

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

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

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

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)

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

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:

$$k_{1}u(A_{1}(u) - B_{1}(u)) = \psi(u)$$
(2.8)

$$A_{1}(u) \exp(-uL_{1}) + B_{1}(u) \exp(uL_{1}) =$$

$$A_{1}(u) \exp(-uL_{1}) + B_{1}(u) \exp(uL_{1}) =$$
(2.0)

$$A_{0}(u) \exp(-u L_{1}) + B_{0}(u) \exp(u L_{1})$$

$$k_{1}u [A_{1}(u) \exp(-u L_{1}) - B_{1}(u) \exp(u L_{1})] =$$
(2.9)

$$k_0 u \left[A_0 \left(u \right) \exp \left(-u \, L_1 \right) - B_0 \left(u \right) \exp \left(u \, L_1 \right) \right]$$
(2.10)

$$A_0(u) \exp\left(-u \left(L_0 + L_1\right)\right) + B_0(u) \exp\left(u \left(L_0 + L_1\right)\right) = 0$$
(2.11)

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

$$A_{1}(u) = \psi(u) \frac{e^{L_{1}u} [k_{1} \sinh (L_{0}u) + k_{0} \cosh (L_{0}u)]}{2k_{1}u [k_{1} \sinh (L_{0}u) \sinh (L_{1}u) + k_{0} \cosh (L_{0}u) \cosh (L_{1}u)]}$$

$$B_{1}(u) = \psi(u) \frac{e^{-L_{1}u} [k_{1} \sinh (L_{0}u) - k_{0} \cosh (L_{0}u)]}{2k_{1}u [k_{1} \sinh (L_{0}u) \sinh (L_{1}u) + k_{0} \cosh (L_{0}u) \cosh (L_{1}u)]}$$

$$(2.13)$$

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:

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

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

with

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

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.



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.,

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

$$= \Pi_0 \exp\left(-\frac{1}{8}u^2w^2\right) \exp\left(-\alpha z\right)$$
(3.1)

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

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

We then have

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

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

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

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

$$T(r, z = L^{+}) - T(r, z = L^{-}) = -R_{c} \left(-k \frac{\partial T}{\partial z}\Big|_{z=L}\right)$$
$$\Delta T(r, L^{-}) = R_{c} \left(-k \frac{\partial \Delta T}{\partial z}\Big|_{z=L}\right)$$
$$\Theta(u, L^{-}) = -R_{c} k \frac{\partial \Theta}{\partial z}\Big|_{z=L}$$

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

$$(3.5)$$

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

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

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

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

$$\Delta T(r,z) = \int_{0}^{+\infty} \left(A(u) \exp(-uz) + B(u) \exp(uz) + \frac{\Pi_{0}}{k(u^{2} - \alpha^{2})} \exp\left(-\frac{1}{8}u^{2}w^{2}\right) \exp(-\alpha z) \right) J_{0}(ru) u \, du$$
(3.8)

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

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

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