

Modeling of the Transient Thermal Response in Solids for Application to IR-PTR

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Introduction:

There are several techniques for the thermal characterization of condensed matter samples, which can be divided in two classes: Steady-state and dynamical methods [1]. Among the later one can mention the Photothermal (PT) techniques [1-2], which are based in the generation and detection of thermal waves. One of the PT techniques which is able to sensing thermal waves directly is the infrared (IR) photothermal radiometry (PTR) technique [2-3]. In the IR-PTR technique, a sample is heated periodically (generally by the absorption of an intensity modulated light beam) and the temperature oscillations are measured as a function of the light modulation frequency at the surface of the sample using an IR radiation detector.

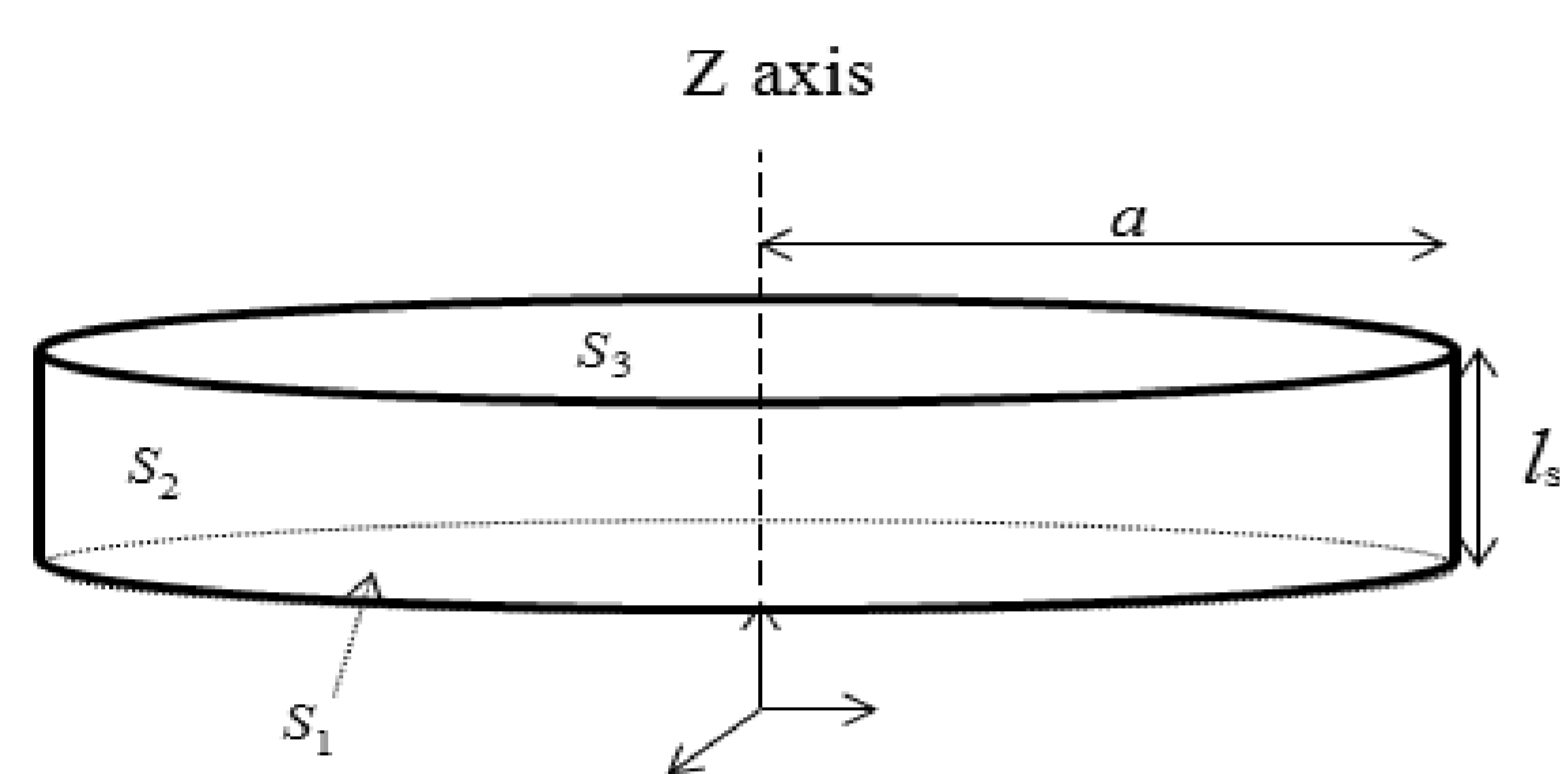


Figure 1. Problem geometry

Computational Methods:

In order to obtain the numerical solution of the eq. (1), restrained by the initial and boundary conditions described by eq. (2), it is necessary to define not only the physical model (equations, and boundary and initial conditions), but also the global parameters (size of the system, modulation frequency, beam waist size, and incident power amplitude), the geometry (coordinate system, symmetries, physical boundaries, etc.), the material properties, and the auxiliary functions (i.e. the power density distribution and the modulation function). For solving the here presented physical problem using CMP, the heat transfer in solids module was employed, in which the dynamical equation is represented by the convection-diffusion equation.

$$\rho C_p \frac{\partial T}{\partial t} + \rho C \vec{u}_p \cdot \nabla T = \nabla \cdot (k \nabla T) + Q \quad (1)$$

In Eq. (1), ρ , C_p and k are the mass density, the specific heat (at constant pressure) and the thermal conductivity of the material, respectively, \vec{u} is the translational motion of the surrounding fluid (here, \vec{u} is assumed to be null); and Q the heat source term. Here, both \vec{u} and Q are assumed to be null, so that for a homogeneous and isotropic sample with constant thermal conductivity the above equation becomes the well-known homogeneous heat diffusion equation. The following boundary conditions have been used for the numerical solution by FEM:

$$\hat{n} \cdot (k \nabla T) + h_{conv} \cdot (T - T_0) + \epsilon_s \sigma_b (T^4 - T_0^4)|_{S_i} = F_i \quad (2)$$

In Eq. (2), the full expression of the Stefan-Boltzmann law was used instead of the linear approximation of the previous section, so that the boundary conditions become non-linear. For the FEM processing, a tetrahedral mesh with two different element sizes was constructed over the domain: One element size was calibrated for “general physics” with a “normal” distribution for the cylinder’s area and the second one using a finer element distribution for both surfaces ($z = 0, l_s$) as showed in Figure 2.

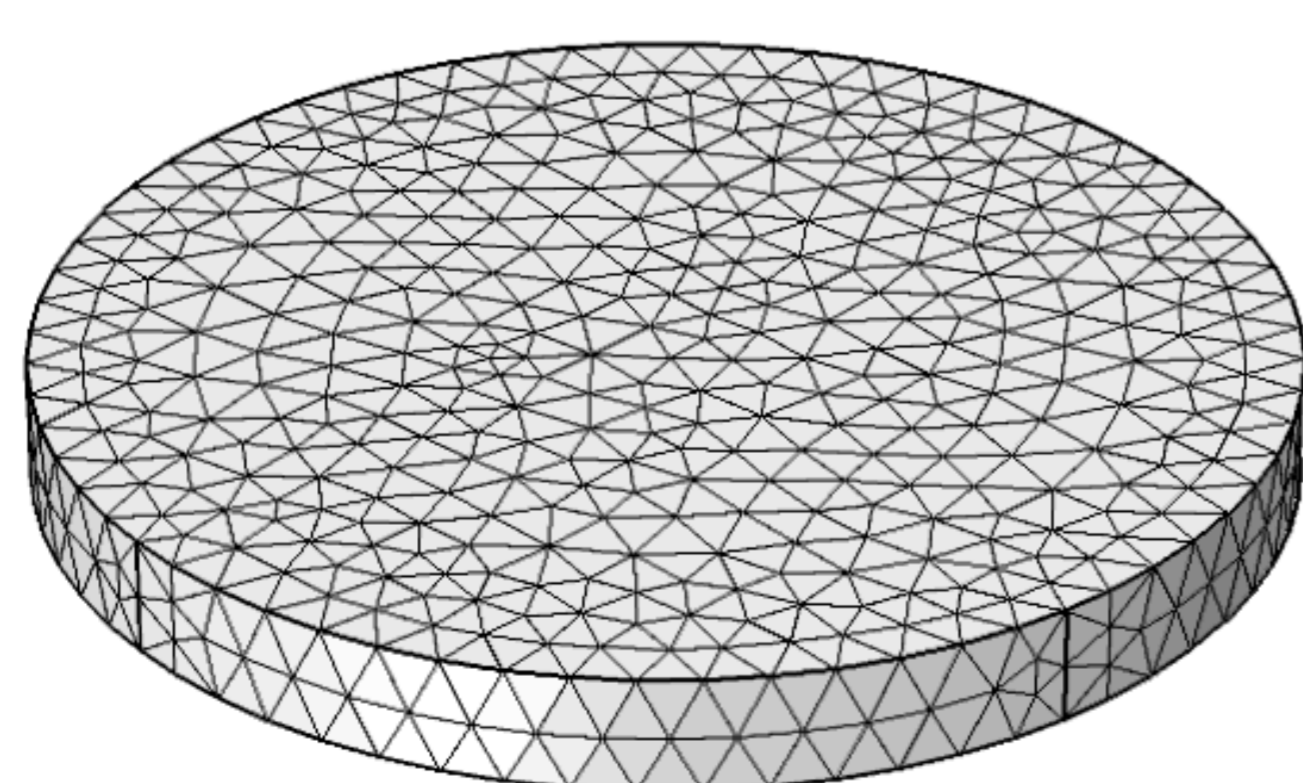


Figure 2. Mesh distribution

Once the model and the meshing were defined, the numerical solver was selected to generate the simulation. In this case, the Fully Coupled solver was chosen, with the BDF (backward differentiation formula) in the strict mode. This allows achieving an accurate convergence for the numerical solution of the PDE involved in the 3D numerical model, obtaining a solution at the edges of the temporal subintervals, during the stipulated simulation time range.

Results:

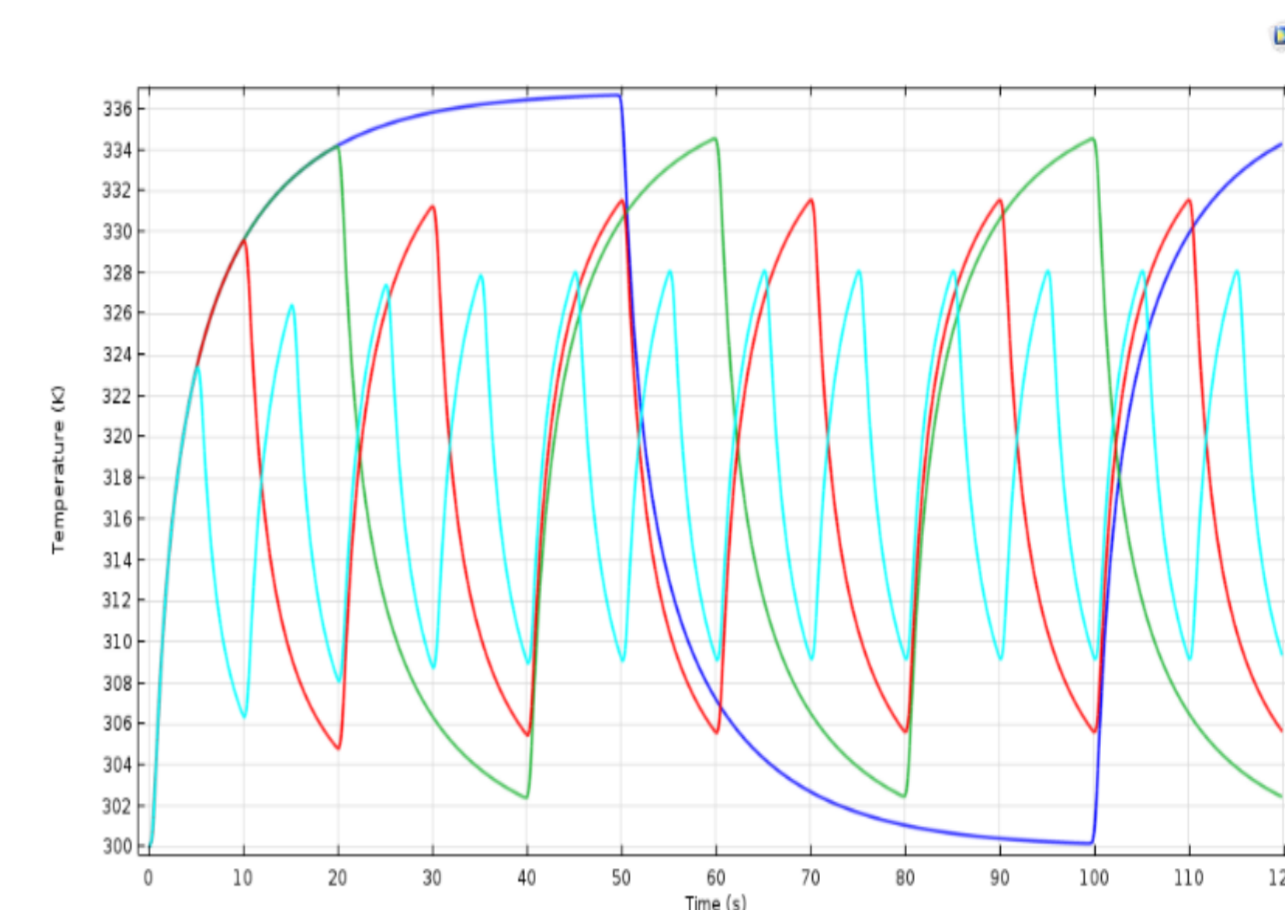


Figure 3. Transient thermal response at different frequencies

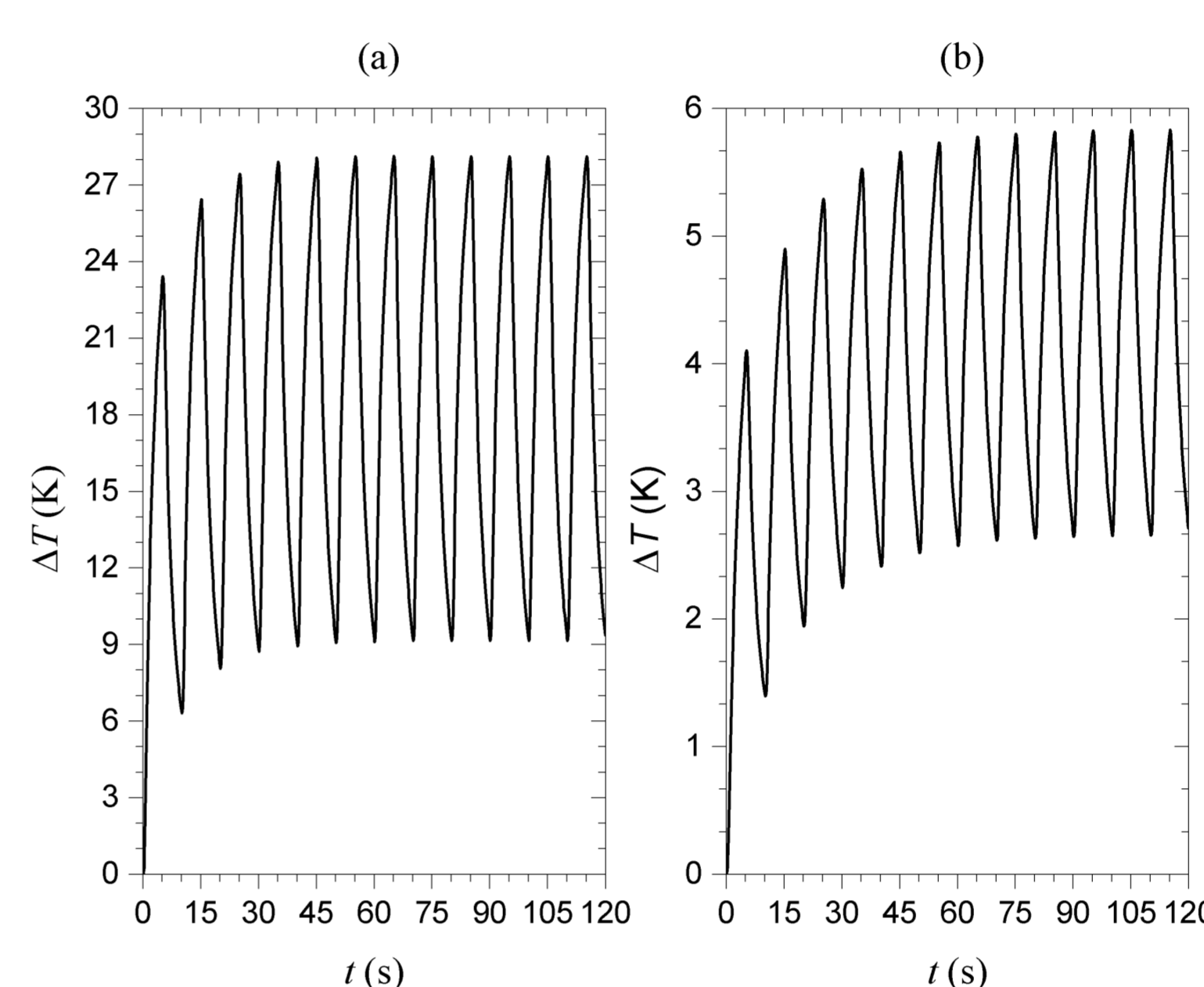


Figure 4.

Figure 4. ΔT calculated at $f = 100$ mHz, for: (a) Balsa Wood, and (b) High Density Polyethylene (HDPE). Here, $\Delta t = 0.1$ s

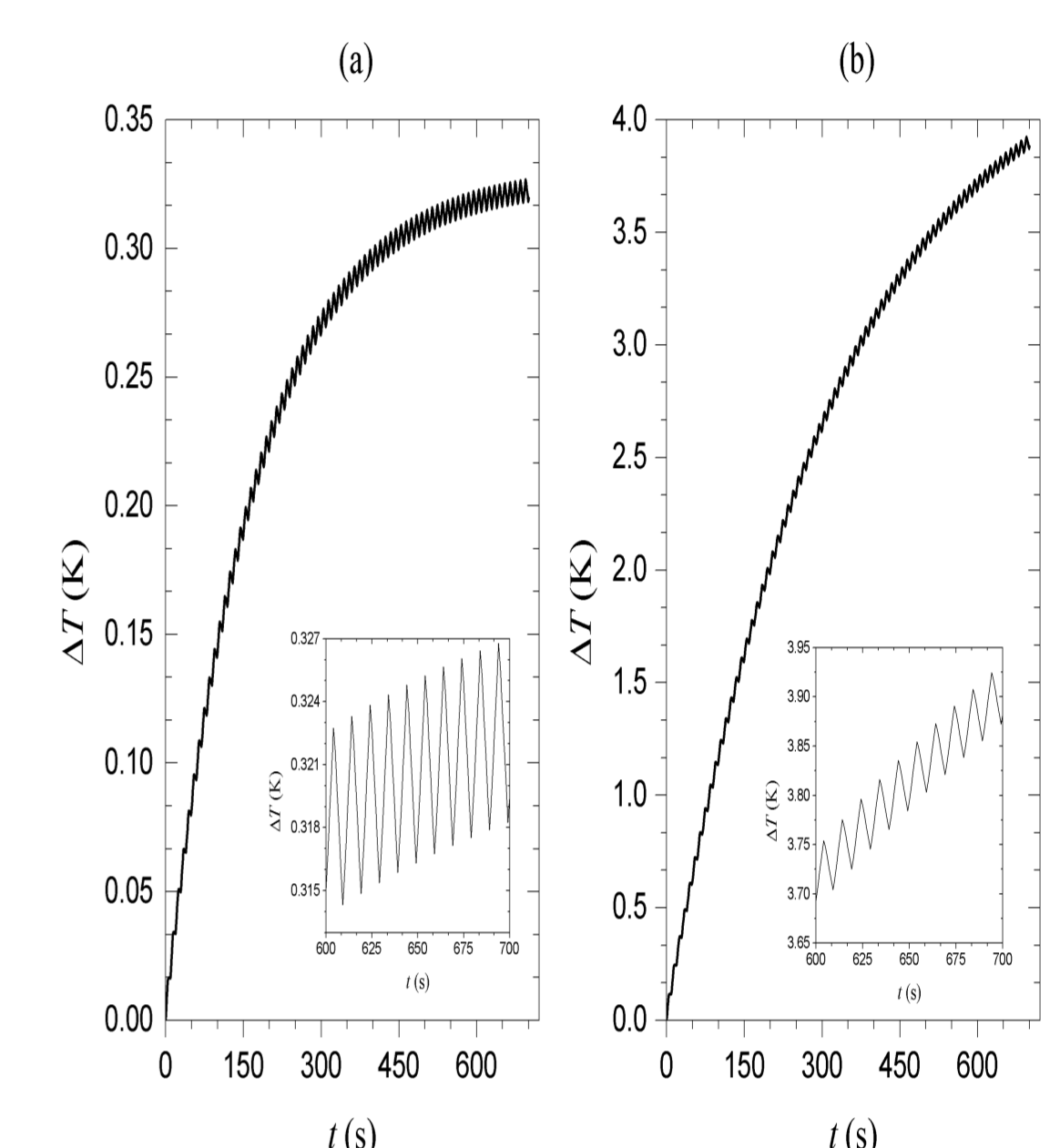


Figure 5.

Figure 5. ΔT calculated at $f = 100$ mHz, for: (a) Al, and (b) Cu. Here, $\Delta t = 1$ s

A comparison between the result obtained by CMP and a theoretical model developed to describe the IR-PTR is shown in figures 6 and 7 for different materials.

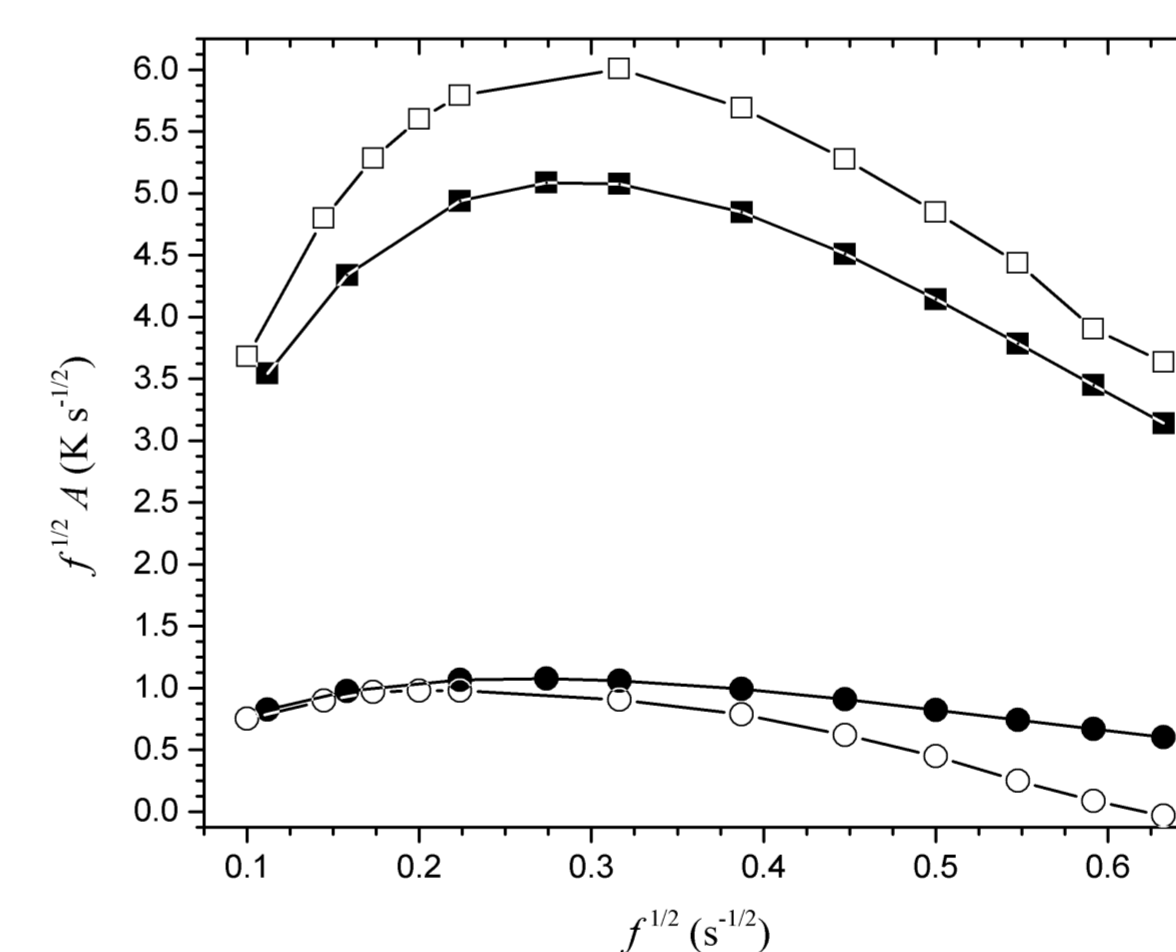


Figure 6.

Figure 6. Amplitudes of the temperature variations, as function of $f^{1/2}$, for: Balsa Wood sample (full circle (t), empty circle (n)), and High Density Polyethylene (HDPE) sample (full square (t), empty square (n)). Here: (t) = theoretical, (n) = numerical.

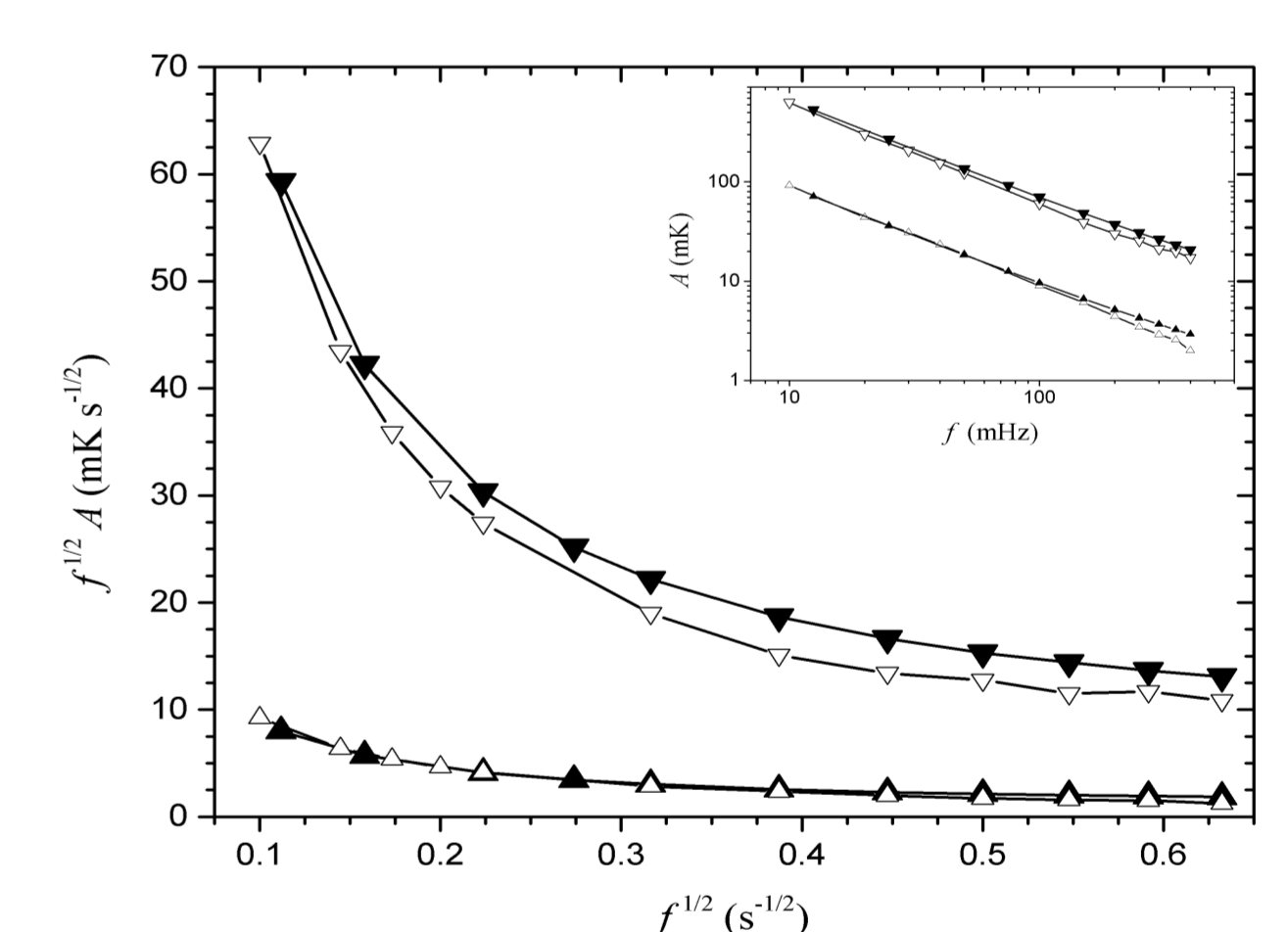


Figure 7.

Figure 7. Amplitudes of the temperature variations, as function of $f^{1/2}$, for: Al sample (full up-triangle (t), empty up-triangle (n)), and Cu sample (full down-triangle (t), empty down-triangle (n)). Here: (t) = theoretical, (n) = numerical

Conclusions:

From the heat diffusion equation, a numerical model considering a monochromatic excitation Gaussian beam, under mixed boundary conditions, were developed to be applied into the study of the transient and oscillatory thermal response in homogenous solids. Such model was capable to reproduce the experimental and theoretical results obtained by the infrared photothermal radiometry.

References:

- [1] D.P. Almond, P.M. Patel, Photothermal Science and techniques, in: Physics and its Applications 10, Chapman and Hall, London, 1996.
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