Thermal and Optical Properties Estimation with the Photoacoustic Spectroscopy and Artificial Neural Networks

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Introduction

The Photoacoustic Spectroscopy (PAS) [1], or more generally the Photothermal Spectroscopy [2,3], are non-destructive testing methodologies that have been applied for the thermal and optical characterization of materials among other applications [2-5].

The photoacoustic effect is the basic phenomenon upon which PAS is built, and it occurs when a material sample placed inside a closed cell filled with air is illuminated with periodically interrupted light. The light absorbed by the sample is converted into heat through a nonradiative de-excitation process. The periodic flow of heat into the air chamber of the cell produces, as an acoustic piston, pressure disturbances in it, which can be detected by a microphone mounted at the cell wall. In the model developed by Rosencwaig and Gersho [6], known as RG theory, this is the only phenomenon taken into account in the PAS signal.

In a previous work [7] we used an implicit inverse problem formulation, and the Levenberg-Marquardt method, for the PAS with the direct problem modeled with the RG theory. As synthetic experimental data it was used only the amplitude of the steady periodic temperature established at the surface of the material sample that is next to the air chamber of the closed photoacoustic cell. We were able to estimate, separately, the thermal diffusivity, α , the thermal conductivity, k , and the optical absorption coefficient, β , of the material under analysis. However, it was not possible to estimate any pair of coefficients simultaneously.

In [8] we extended our previous results by considering also as experimental data the phase-lag between the temperature at the sample-gas interface and the modulated light source. An improvement on the solution of the inverse problem was observed (smaller confidence bounds) when each parameter was estimated separately, except for the thermal conductivity, due to the null sensitivity of the phase-lag with respect to this parameter. The simultaneous estimation of (α,β) was performed but the estimated values for the unknowns were corrupted by the amplification of the error present in the experimental data.

In [9] a one parameter family of regularization terms constructed with Bregman distances based on the *q*-discrepancy function was implemented in the formulation and solution of PAS as an inverse problem. The original idea was improved by the proper weighting of the unknowns to be determined. We have focused on the simultaneous estimation of the sample thermal diffusivity, α , and optical absorption coefficient, β . The results were significantly improved in comparison to our previous works [7,8].

In the present work we use Artificial Neural Networks for the estimation of the thermal diffusivity of a reference material [10].

Direct Problem

In a cylindrical closed photoacoustic cell the sample of the material under analysis is placed upon a backing material, and the other boundary of the sample adjoint to the air chamber of the cell, is exposed to an incident modulated light with intensity

$$I(t)=\frac{1}{2}I_0\left(1+\cos\omega t\right) \tag{1}$$

where I_0 is the maximum intensity of the incident light, and ω is the angular frequency of the chopping mechanism.

It is assumed that the light doesn't go through any interaction within the air chamber and is fully absorbed by the material sample according to Beer's law

$$I_s(x,t) = e^{\beta x} I(t) \quad (2)$$

where β is the optical absorption coefficient.

The volumetric heat generation at the sample due to the light absorbed is given by

$$S(x,t) = \frac{dI_s(x,t)}{dx} = \frac{1}{2}\beta I_0 e^{\beta x}(1+\cos \omega t) \quad (3)$$

If we know the optical and thermal properties of the sample, the thermal properties of the other materials in the photoacoustic cell, the physical dimensions of the backing material, sample and air chamber, the frequency of the chopping mechanism, and the intensity of the incident light, then from the heat conduction problem in the photoacoustic cell we calculate the values for the amplitude and phase-lag of the temperature at the interface sample-gas between the material and the air chamber [6,9].

Inverse Problem

In the present work we considered the inverse problem of estimating the thermal diffusivity of a reference material with an Artificial Neural Network [10].

In Fig. 1 is shown the error in the training stage of the neural network as a function of the epoch. Each epoch represents the presentation of the full set of patterns used in the training. The patterns consisted on the amplitude and the phase-lag of the temperatures at the sample-gas interface.

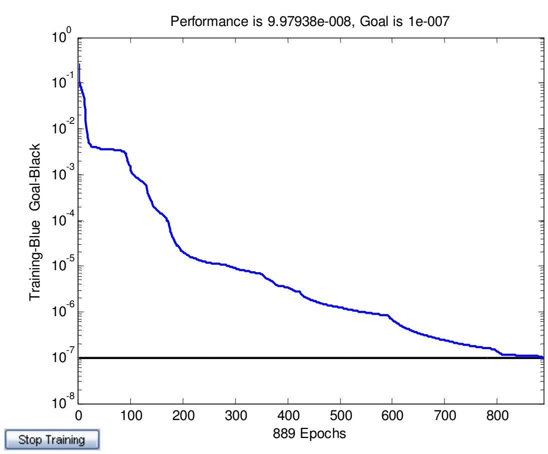

Figure 1 - Error in the training stage of the Artificial Neural Network.

Conclusions

From the sensitivity analysis we could forecast that the simultaneous estimation of the thermal and optical properties is a difficult task. Such difficulty was also confirmed in our previous works. Therefore, we have opted in the present work to estimate only one parameter, the thermal diffusivity. The Artificial Neural Network developed for that purpose was very successful.

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