Photothermal depth profiling for multilayered Structures by particle swarm optimization

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Abstract. This paper presents a method to reconstruct thermal conductivity depth profile of a layered medium using noisy photothermal data. The method tries to obtain an accurate reconstruction of discontinuous profile using particle swarm optimization (PSO) algorithm and total variation (TV) regularization. The reconstructions of different thermal conductivity profiles have been tested on simulated photothermal data. The simulation results show that the method can find accurately the locations of discontinuities, and the reconstructed profiles are in agreement with the original ones. Moreover, the results also show the method has good robustness and anti-noise capability.

1. Introduction
In recent years photothermal techniques have been applied to investigate thermal conductivity depth profiles of inhomogeneous samples [1,2]. In order to characterize such samples one may generate a plane thermal wave at sample surface by using a pump beam modulated at the frequency $f$. The quantity $f$, which is adjustable, drives the penetration depth of the thermal wave used for the investigation. Noninvasive thermal-wave imaging of depth profiles is very appealing in several areas from civil and industrial engineering to nondestructive testing and biomedical applications. In spite of this great importance, most thermal-wave imaging techniques are still far from solving practical problems. In fact, there are theoretical aspects hard to manage, such as, the nonlinear and non convex relationship between the thermal-wave field and the object structure, the robustness of the inversion algorithms against noise. Working on an ill-posed problem, photothermal inversion normally provides either unstable or oversmoothed results. Recently, evolutionary computing methods such as genetic algorithms (GA) [3] and particle swarm optimizations (PSO) [4] have been tried in continuous profile reconstruction problems, and these approaches proved to be able to efficiently find a global optimum in a fitness landscape.

In this paper, reconstructions for discontinuous and step-index thermal conductivity profiles are attempted by using PSO algorithm and total variation regularization. The specific problem regards the reconstruction of thermal conductivity profile of a multilayer slab from measurements of the alternating temperature of the object surface within a certain frequency range. Some details on the formulation of the profile reconstruction problem are given, and several reconstruction simulations are performed to evaluate the capability of the inversion method to find the locations of discontinuities. Moreover, the influences of noise on the reconstruction results are also investigated.
2. Particle swarm optimization implementation

The sample considered here is a multilayer slab, which located on a semi-infinite homogeneous substrate. For charactering the thermal properties of the slab, a modulated plane heat source is located at the sample surface. Then the amplitude and phase of surface alternating temperature is measured at $m$ modulated frequencies $f_m$ within the chosen frequency range. The aim is to estimate the thermal conductivity of the slab as a function of the depth coordinate $z$. To solve this problem, the slab is discretized into a finite number $N$ of homogeneous layers. Then the photothermal signal is calculated as follows: $S=Z_i S_{ref}=A \exp(i \phi)$, where $S_{ref}$ is the reference signal of a homogeneous sample, and $Z_i$ is the surface thermal impedance calculated, layer by layer ($n= N…1$), by the following recursive formula [1,4]:

$$Z_n = \frac{\cosh(q_m h_n) + \frac{1}{k_n q_m} \sinh(q_m h_n)}{k_n q_m \sinh(q_m h_n) Z_{n+1} + \cosh(q_m h_n)}.$$

(1)

where $q_m=(2\pi f_m c/\kappa)^{1/2}$, $\kappa$, $h_n$ are thermal wave vector, thermal conductivity, thickness, of the $n$th layer, respectively. $\rho$ and $c$ are density and heat capacity of the slab.

The inversion algorithm has to find the configuration of layers that gives the best fit between the measured and the computed photothermal signals, subject to suitable regularizing constraints. The forward solver implemented in the code evaluates the photothermal signals of any structure composed by a finite number of layers for each of the $m$ frequencies $f_m$. The minimized fitness function to be optimized is the following:

$$F(k) = \left[ \sum_{m=1}^{m} (S_{teo}(f_m, k) - S_{exp}(f_m, k)) \right]^{1/2} + \lambda \sum_{n=1}^{N-1} |k_{n+1} - k_n|.$$

(2)

where the first term in equation 2 is a suitable distance between the two $m$-element arrays of the experimental ($S_{teo}$) and the theoretical ($S_{exp}$) photothermal signals (amplitudes or phases). The second term is the total variation (TV) regularization function [5], which is appropriate for problems where we except there to be discontinuous jumps in the model. Hyper-dimensional vector $k = (k_1, k_2, \ldots, k_N)$ represents the reconstructed conductivity profile and $\lambda$ is the regularization parameter. The equation 2 is non-convex, and a global optimization is required to converge to the minimum. A particle swarm optimization (PSO) algorithm [6] is adopted to optimize equation 2 since this approach has proved to be reliable and efficient in the smooth profile reconstruction problems [4].

PSO starts with the random initialization of a population of individuals (particles) in the search space and works on the social behaviour of the particles in the swarm. Each particle is treated as a mass-less and volume-less point in a $D$-dimensional space. The $i$th particle is represented as $x_i = (x_{i1}, x_{i2}, \ldots, x_{id})$. The best previous position of the $i$th particle that gives the best fitness value is represented as $p_i = (p_{i1}, p_{i2}, \ldots, p_{id})$. The best particle among all the particles in the population is represented by $p_g = (p_{g1}, p_{g2}, \ldots, p_{gd})$. Velocity, the rate of position change for the $i$th particle, is represented as $v_i = (v_{i1}, v_{i2}, \ldots, v_{id})$. At every iteration, the velocity and the position of each particle are updated by using the two best values according to the following equations:

$$v_{id}^{t+1} = \omega \cdot v_{id}^{t} + c_1 \cdot r_1 \cdot (p_{id}^{t} - k_{id}^{t}) + c_2 \cdot r_2 \cdot (p_{gd}^{t} - k_{id}^{t}).$$

(3)

$$x_{id}^{t+1} = x_{id}^{t} + v_{id}^{t+1}.$$

(4)

Here $t$ is the iteration number, $d = 1, 2, \ldots, D$, $i = 1, 2, \ldots, S$, and $S$ is the size of the population. $\omega$ is the inertial weight factor, $c_1$ and $c_2$ are acceleration constants, $r_1$ and $r_2$ are two random numbers uniformly distributed in the interval $[0, 1]$. In the PSO inversion, a particle represents a possible thermal conductivity profile $k (D = N)$, and the choice of $k$ is determined by the intrinsic relationship between the photothermal signal and the thermal conductivity profile. In each epoch of the optimization routine, the cost function is calculated by equation 2, and the repeated application of equation 3 and 4 leads to the evolution of the population towards the best solution.
In this study, the PSO population size $S$ is 30, the inertial weight $\omega$ is linearly decreasing from 0.9 to 0.4 during the iterations, the acceleration constants $c_1$ and $c_2$ are equal to 2, and the maximum velocity $v_{\text{max}}$ is set to 0.1 times of the maximum particle position. Moreover, the maximum iteration number (epoch) for training is 4000, which is selected based on the convergence rate of the inverse problem. Moreover, the criterion to select the best regularization parameter $\lambda$ is given by looking at the edge of L curve in the $\chi^2$ fit [5].

3. Discussion of simulation results

![Figure 1](image1.png)

Figure 1. Reconstructed results for thermal conductivity profile with the same layer thickness: (a) simulated phase signals and fitted results; (b) reconstructed profiles for different noisy data.

![Figure 2](image2.png)

Figure 2. Reconstructed results for thermal conductivity profile with different layer thickness: (a) simulated phase signals and fitted results; (b) reconstructed profiles for different noisy data.

To assess the inversion procedure we have initially used simulated data to test the reliability of the results from structures with exactly known features. For simplicity, we considered the slab has a depth independent specific heat capacity 480 J Kg$^{-1}$ K$^{-1}$ and density 7700 Kg m$^{-3}$. In the inversion, the bandwidth of the modulation frequency used for profile recognition is of major importance. Here, the method introduced in Ref [7] is used to select a reasonable frequency range. Figure 1 shows a typical result of the inversion method for reconstructing a three-layer profile with the same layer thickness, where $N = 15$ virtual layers and $M = 108$ frequencies in the range 1 Hz – 400 Hz is used. Figure 1(a) shows the simulated phase signals of SNR = 20 dB (circle) and 10 dB (triangle) and corresponding fitted results using PSO optimization (solid line: for phase signal with SNR = 20 dB; dotted line: for phase signal with SNR = 10 dB), where good fitted results still can be observed when signal noise is relatively larger. Figure 1(b) shows the reconstructed profiles (dash line of circles: for phase signal
with SNR =20 dB; dotted line of triangles: for phase signal with SNR = 10 dB) in comparison with the
original profiles (solid line). Figure 1(b) indicates clearly that the reconstruction results are quite
satisfactory, where the discontinuous position of profile can be found clearly and the reconstructed
profiles are in agreement with the original ones. Moreover, it can be found that the noise increase only
decreases slightly the precision the reconstructed profile, so the algorithm is very robust to noise.
Figure 2 shows the reconstructed result for a three-layer thermal conductivity profile with different
layer thickness ($N = 20$). It can be found that the results of reconstructed profiles for different noisy
data are still quite good.

![Figure 3](image)

**Figure 3.** Reconstructed results obtained in a case where the discontinuity lines do not match the
reconstruction grid.

To show how the choice of virtual layer number is not a critical point, a case when the simulation
and the reconstruction grids are different is shown in figure 3 ($N = 20$), where the true profile is the
same to that in figure 1. It can be found that, although the discontinuities in the original profile do not
fit the reconstruction lattice cells, the positions of discontinuity still can be located very well within
the resolution allowed by the reconstruction grid.

4. Conclusion

In this paper, based on particle swarm optimization and total variation regularization, we have
presented a reliable inversion method for photothermal depth profiling of multilayered structures. The
reconstructions of the thermal conductivity profiles have been tested on different simulated phase data.
The simulation results show the method has good resolution and robustness against noise. Moreover,
the ability of the inversion method to detect and locate discontinuities is rather satisfactory. It should
be mentioned that reconstructing depth profiles of thermal conductivity from photothermal amplitude
data is also feasible by using the inversion method.

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