Analysis of the Tikhonov regularization to retrieve thermal conductivity depth-profiles from infrared thermography data

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(Received 2 June 2010; accepted 3 July 2010; published online 20 September 2010)

We analyze the ability of the Tikhonov regularization to retrieve different shapes of in-depth thermal conductivity profiles, usually encountered in hardened materials, from surface temperature data. Exponential, oscillating, and sigmoidal profiles are studied. By performing theoretical experiments with added white noises, the influence of the order of the Tikhonov functional and of the parameters that need to be tuned to carry out the inversion are investigated. The analysis shows that the Tikhonov regularization is very well suited to reconstruct smooth profiles but fails when the conductivity exhibits steep slopes. We check a natural alternative regularization, the total variation functional, which gives much better results for sigmoidal profiles. Accordingly, a strategy to deal with real data is proposed in which we introduce this total variation regularization. This regularization is applied to the inversion of real data corresponding to a case hardened AISI1018 steel plate, giving much better anticorrelation of the retrieved conductivity with microindentation test data than the Tikhonov regularization. The results suggest that this is a promising way to improve the reliability of local inversion methods. *© 2010 American Institute of Physics*.
[doi:10.1063/1.3475498]

I. INTRODUCTION

Over the last decades, a great deal of effort has been devoted to develop nondestructive tests to evaluate the hardness profile of case hardened steels. Photothermal radiometry, which is a well known tool for the measurement of thermal properties of matter, has emerged as a promising technique in this area, since several works have assessed an anticorrelation between hardness and thermal conductivity of the hardened steels.[1–4] Under this approach, the reconstruction of the hardness profile turns into the reconstruction of the thermal conductivity profile. However, the inverse problem of reconstructing thermal conductivity profiles of case hardened steels from infrared radiometry data suffers from ill-posedness, i.e., rather different thermal conductivity profiles give quite similar surface temperature, amplitude, and phase spectra, within experimental uncertainty. For this reason, the reconstructed profiles are extremely sensitive to noise in the data.

The ill-posed character of the inverse problem increases with the number of unknowns. Accordingly, a possible approach consists in reducing the number of unknowns by assuming a predetermined functional form of the conductivity profile, depending on few parameters.[1,5–7] Of course this restricts the shape of the retrievable conductivity profile to that of the selected function. In this way, more sophisticated versions of this approach have been developed, in which the parameters defining the function are recalculated for the increasing depths corresponding to decreasing frequencies.[8] On the other hand, the number of unknowns can also be reduced by assuming a multilayer model for the thermal conductivity profile and using only a few layers for the reconstruction. The drawback of this solution is related to the lack of spatial resolution of the reconstruction.

The approaches described in the previous paragraph consist in avoiding the ill-posedness of the problem by assuming very significant qualitative and quantitative *a priori* knowledge about the shape of the conductivity profile, at the price of reducing the information one can attain from the photothermal data. However, in the case where spatial resolution is to be obtained without restrictions on the functional form of the conductivity profile, the full ill-posedness of the problem needs to be faced. From a mathematical point of view this means that the solution is not unique and/or is not stable (small perturbations in the data cause substantial changes in the solution). In general, finding the solution consists in obtaining the model parameters which minimize the residual function (a function of the squared differences between experimental and calculated data). However, if the inverse problem is ill-posed and nonlinear, it may exhibit several minima, global, and/or local. The minimization process suffers from instability and regularization procedures need to be applied. The methods developed to find the solution (minimum of the residual) can be classified into two categories: global methods and local methods. Global methods like genetic algorithms,[9] neural networks,[10,11] or more recently, particle swarm optimization,[12] look for global minima by trying over wide ranges of parameter values, while local methods start from a certain set of parameter values and modify them in an controlled way until the minimum of the residual is reached. In general, if some information about the properties of the function to be minimized is known, local methods are

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preferable because of the big amount of evaluations of the goal function that the global models need to deal with. Moreover, local methods reach the parameters which minimize the residual more accurately than global methods do.

Among local methods, the Tikhonov regularization procedure has been successfully applied to the reconstruction of thermal conductivity depth-profiles of case hardened steels.[4,13] In this problem, although a global minimum (the solution) exists, it is not stable. The method consists in adding a stabilization term to the residual. This term contains a regularization functional multiplied by a regularization parameter, which determines the size of the whole regularization term. The choice of this regularization parameter can be made in different ways. One possibility is using the L-curve method;[14] however, a certain ambiguity appears in the choice of the right regularization parameter associated to the location of the L-corner, since several values might look like possible right regularization parameters. A second possibility consists in using an iterative method in which the regularization parameter is reduced at each iteration, and stopping the process at the first iteration where the residual is of the order of the experimental noise (Morozov discrepancy principle).[15] Unlike in the L-shape method, here the noise level is required as prior information. It is worth mentioning that establishing the stopping criterion as a function of the noise in the experimental data avoids overfitting of the data (fitting the noise rather than the underlying function). The Tikhonov regularization procedure has given quite good results in the reconstruction of conductivity depth-profiles, qualitatively anticorrelated with the results of microindentation tests.[4,13] However, the conductivity profiles are systematically smoother than the microhardness profiles, especially in the deeper regions, showing an apparent penetration deeper than the actual case depth.[4,13]

In this work we analyze the accuracy of the Tikhonov regularization procedure to retrieve thermal conductivity profiles depending on the functional form, the smoothness and the depth of the characteristic conductivity variation, as well as on the noise of the experimental data. In particular, we will reconstruct shapes that are often encountered in hardened materials: exponential, oscillating, and sigmoidal profiles.[3,8,13] First, for each conductivity profile we generate synthetic amplitude and phase data which are calculated by applying the thermal quadrupole method with a high number of layers. Then we add white noise to simulate experimental data. Systematic errors are only considered in the case they result in a homogeneous factor in amplitude and a shift in phase. We will examine the influence of the order of the Tikhonov regularization function and of the associated initial guess on the quality of the final reconstruction. The results will show that the Tikhonov regularization gives excellent results for smooth profiles but starts failing when retrieving steep profiles. We propose to use a total variation regularization functional when the results of Tikhonov regularization give failure signs. We suggest a full strategy for addressing the case of a real problem and we apply it to real data. The good agreement between the reconstruction and microhardness test data is very promising regarding the development of reliable local inversion methods.

II. THE TIKHONOV REGULARIZATION PROCEDURE

The problem we are dealing with consists in retrieving the thermal conductivity profile of hardened materials from infrared thermography data, when the sample is illuminated with a flat light beam, modulated at frequency f. In case hardened steels, the hardening process reduces the conductivity at the surface if compared with the conductivity of the unhardened material. The hardening penetration is typically of 0.5–2 mm, and deeper inside the material the thermal properties remain unchanged. In other systems, like cured dental resins, the photopolymerization process leads to a higher thermal conductivity in the cured than in the raw resin,[16] so we will study thermal conductivity profiles of both, increasing and decreasing values in depth. According to previous experimental results,[3] in this paper we assume that the heat capacity (ρc) is constant along the hardened region.

In order to solve the direct problem (calculation of the surface temperature amplitude and phase as a function of the modulation frequency) for a certain profile we apply the thermal quadrupole method.[17] In this approach, the continuously varying thermal conductivity is approximated by a layered and opaque structure, made on N parallel layers of thicknesses l_j, thermal conductivities K_j, and equal heat capacity ρc. This method allows fast and reliable calculation of the surface temperature amplitude and phase. For the direct calculation of the temperature we have used 4000 layers, guaranteeing that the surface temperature data as a function of the modulation frequency are exact.[4] Both amplitude and phase are sampled in $M=60$ frequencies equally spaced in a logarithmic scale in the range $0.1-10^4$ Hz. The calculated amplitude and phase are finally normalized to the values of an unhardened sample. Then we add white noise by adding to the calculated amplitudes and phases two "noise vectors" whose M entries are random values between $+\varepsilon_A$ and $-\varepsilon_A$ for amplitude, and $+\varepsilon_\psi$ and $-\varepsilon_\psi$ for phase. In the cases where we want to simulate typical experimental noise for this kind of measurements, we set $+\varepsilon_A=0.025$ to represent $\pm 2.5\%$ noise in normalized amplitude, and $+\varepsilon_\psi=0.5°$ in normalized phase. Then we invert the data using a very different number of layers, N, than in the direct problem. Although for the sake of simplicity we usually make $M=N$, to maintain generality, we will retain, both M and N along the text. Using different schemes for solving the direct and inverse problems is mandatory to avoid inverse crimes, i.e., an excessively optimistic accuracy of the reconstruction.[18]

In a previous work, we presented some improvements that we introduced in the Tikhonov regularization procedure to retrieve thermal conductivity profiles of case hardened steels from infrared thermography data.[4] These improvements include a renormalization of the data, a frequency weighting, and the simultaneous fitting of the amplitude and phase data contained in a single function. Our model also deals with systematic errors usually encountered in experimental data, leading to a factor in amplitude and a shift in phase. We remove these constants from the experimental and calculated data by performing a renormalization in the following way: according to the frequency weighting, we calculate the norm of all the amplitude values (A) and the mean of all the phase values (ψ).[4] Then, each amplitude is divided by the norm of the amplitudes and the mean of all phases is subtracted to all the phase values.

All these improvements can be condensed in a residual function r of the conductivity functions K that writes as follows:[4]

$$\begin{aligned} r(K) & \int_0^\infty \frac{[A_{N_{the}}(f) - A_{N_{\exp}}(f)]^2}{f[\beta + \log^2(f)]} df \\ & + \gamma^2 \int_0^\infty \frac{[\psi_{N_{the}}(f) - \psi_{N_{\exp}}(f)]^2}{f[\beta + \log^2(f)]} df \\ & = \int_{-\infty}^\infty \frac{[A_{N_{the}}(u) - A_{N_{\exp}}(u)]^2}{\beta + u^2} du \\ & + \gamma^2 \int_{-\infty}^\infty \frac{[\psi_{N_{the}}(u) - \psi_{N_{\exp}}(u)]^2}{\beta + u^2} du, \end{aligned} \tag{1}$$

where f represents the frequency, A_{Nthe} and $A_{N\,exp}$ are the calculated and measured renormalized amplitudes, respectively, ψ_{Nthe} and $\psi_{N\,exp}$ are the calculated and measured renormalized phases, respectively, β is a constant added to overcome the divergence introduced by the square logarithm at $f=1$ Hz, $u=\log(f)$, and the factor γ is introduced to balance the noise levels of the two quantities, amplitude and phase, that we are combining for the minimization.[4] In our problem, the frequency (f) and the conductivity (K) do not correspond to continuous functions, but to discrete values of the experimental frequencies and of the conductivities of all the layers, respectively, so the expression of $r(K)$ needs to be discretized. Moreover, a regularization term needs to be introduced in order to stabilize the minimization process. We will use the Tikhonov regularization term. Taking all this into account, the final form of the function $r_\alpha(K)$ to be minimized is:[4]

$$\begin{aligned} r_\alpha(K_1, \ldots, K_N) = \alpha J(K_1, \ldots, K_N, K_1^0, \ldots, K_N^0) + \sum_{i=1}^{M} \frac{[A_{N_{theoc}}(K_1, \ldots, K_N, u_i) - A_{N_{\exp}}(u_i)]^2}{\beta + u_i^2} \Delta u_i \\ + \gamma^2 \sum_{i=1}^{M} \frac{[\psi_{N_{theo}}(K_1, \ldots, K_N, u_i) - \psi_{N_{Exp}}(u_i)]^2}{\beta + u_i^2} \Delta u_i. \end{aligned} \tag{2}$$

The second and third terms of the right-hand side are the discrete version of the residual, r, usually called the discrepancy term, and the first term is the Tikhonov penalty term,[19] being J the Tikhonov penalty functional, $\alpha > 0$ the regularization parameter, and K_j^0 with $j=1, \ldots, N$ an initial guess of the conductivities of all the layers. Note that, for frequencies equally spaced in a logarithmic scale Δu_i is the same for $i=1 \ldots M$, which simplifies the calculations.

The Tikhonov penalty term contains two contributions: the regularization parameter, α, determines the size of the penalty term, and the Tikhonov penalty functional J, which, together with the initial guess K_j^0 ($j=1, \ldots, N$), penalizes any conductivity profile different from the one described by the full penalty term.

Regarding the Tikhonov penalty functional, several orders of this functional can be used to stabilize the minimization process. The so-called "zero order" or standard Tikhonov penalty term,

$$J(K_1, \ldots, K_N, K_1^0, \ldots, K_N^0) = \sum_{j=1}^{N} l_j (K_j - K_j^0)^2, \tag{3}$$

penalizes conductivity profiles very different from the initial guess, K_j^0 ($j=1, \ldots, N$). The "first order" Tikhonov penalty functional with a Dirichlet boundary condition on the deepest layer,

$$\begin{aligned} & J(K_1, \ldots, K_N, K_1^0, \ldots, K_N^0) \\ & \quad = \sum_{j=1}^{N-1} \frac{1}{l_j} [(K_{j+1} - K_j) - (K_{j+1}^0 - K_j^0)]^2 \\ & \quad + \frac{1}{l_N} (K_{\text{unhardened}} - K_N)^2, \end{aligned} \tag{4}$$

penalizes conductivity profiles with derivatives which are different from the derivative of the initial guess; in addition the conductivity of the deepest layer must be close to the conductivity of the unhardened material. Higher order Tikhonov penalty terms look for the similarity between the successive derivatives of the retrieved and initial conductivity profiles. This indicates that: (a) the Tikhonov penalty term allows introducing prior information about the problem and (b) the higher the order of the function, the smoother the retrieved conductivity profile will be. The availability of prior information and the possibility of introducing it in the minimization procedure are crucial for retrieving meaningful conductivity profiles. From a physical point of view, the reason for this is that, since thermal waves are heavily damped, information from deep inside the material barely reaches the surface, where data are taken, so some information about the conductivity deep inside the material is needed.

Regarding the regularization parameter, as mentioned in the previous section, instead of keeping it constant during the minimization, we have implemented a Newton-type iterative algorithm, suggested by Bakushinskii,[20] allowing to introduce the regularization term. In this algorithm, we reduce the regularization parameter at each iteration and we apply the Morozov discrepancy principle, stopping the process when the residual is of the order of the noise level of the experiment. Briefly speaking, in each iteration a reconstruction of the thermal conductivity K_j $(j=1,\ldots,N)$, is retrieved by solving a linear system of equations, using continuously decreasing α values, according to $\alpha_{n+1}=\eta\alpha_n$ with $\eta\in(0,1)$. The initial value of α needs to be high enough so that the whole stabilization term is, at least, of the same order of magnitude as the initial residual. The reduction factor η governs the rate of convergence: the lower the η value, the faster the rate. However, a too small η value might reduce the stabilization introduced by the Tikhonov's penalty term too fast. In this work we have set $\eta=0.5$.

III. NUMERICAL CALCULATIONS AND DISCUSSION

In this section we present the results of conductivity profiles obtained using the method described above. As mentioned in the previous section, we have generated amplitude and phase data using 4000 layers in the direct problem and have set $+\varepsilon_A=0.025°$ and $+\varepsilon_\psi=0.5°$ in the noise vectors corresponding to the amplitude and phase, respectively, to simulate the typical experimental noise level in infrared thermography data. We analyze the ability of the method to retrieve conductivity profiles of three different shapes (exponential, oscillating and sigmoidal), characterized with different depths and smoothness of their characteristic variation. For this purpose, we have used both, zero order and first order Tikhonov functions. Concerning the initial value of the regularization parameter, we start by setting its standard value (α_0) of the same order of magnitude as the initial discrepancy term. If this standard value does not lead to convergence, we increase the value of the initial regularization parameter by multiplying α_0 by successive increasing factors until convergence is reached. As will be shown below, this optimum factor depends on the choice of the initial guess. Finally, we study the effect of the noise in the data on the quality of the final reconstruction. In order to give the resulting final reconstruction for a certain noise level, we let the position of the unhardened layer to be located at different depths, namely, 0.8, 1, 1.2, 1.4, 1.6, and 1.8 mm. In all the simulations the conductivity of the unhardened material is 50 $\mathrm{Wm^{-1}\,K^{-1}}$. We add different random noise vectors, all having entries between the same extreme values, $\pm\varepsilon_A$ for the amplitude, and $\pm\varepsilon_\psi$ for the phase. Then we start from three different initial guesses: constant 50 $\mathrm{Wm^{-1}\,K^{-1}}$ conductivity, decreasing linear profile with a conductivity of 75 $\mathrm{Wm^{-1}\,K^{-1}}$ at the surface, and increasing linear profile with a conductivity of 25 $\mathrm{Wm^{-1}\,K^{-1}}$ at the surface. Note that, although the value of the conductivity is known deep inside the material, the precise depth at which the case hardening has no longer penetrated is unknown. From all the reconstructions we calculate the mean conductivity value for each depth and we assign the corresponding error bar.

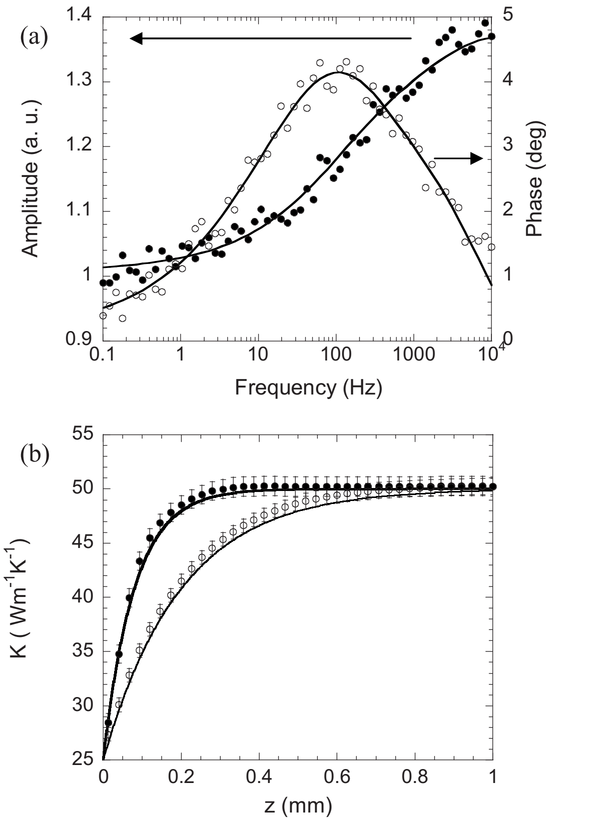

FIG. 1. (a) Amplitude (dots) and phase (circles) data with added white noise corresponding to the conductivity profile depicted by a thick line in Fig. 1(b), together with the fittings (solid lines) and (b) real (lines) and reconstructed (symbols) exponential conductivity profiles obtained from calculated data with added white noise similar to our experimental noise. The symbols represent the mean value of the conductivity retrieved at each depth from different initial guesses, noise vectors and bulk conductivity depths

A. Exponential profiles

The first profile we have analyzed is the exponential one. We have studied steep and smooth, both increasing and decreasing exponential profiles. First, we have checked the influence of the order of the Tikhonov functional. For this type of profile zero and first order Tikhonov functionals lead to very similar reconstructions, although the first order functional yields slightly better results. The influence of the initial value of the regularization parameter is also small. Actually, variations in this parameter of several orders of magnitude have very slight influence on the final result. As an example, in Fig. 1(a) we show synthetic amplitude (dots) and phase (circles) data with added white noise similar to the experimental noise together with the fittings (solid lines) corresponding to the conductivity profile depicted by a thick line in Fig. 2(b). Here, in Fig. 2(b), two true conductivity profiles with different exponential factors are shown together with the reconstructed profiles (dots for the steepest profile and circles for the smoothest one) including the uncertainty bars. As can be observed, the reconstructions are excellent. The uncertainty in the reconstructions increases with increasing depth and corresponds to about 1% at the surface and about 2% at 1 mm depth. Similar results were obtained for exponential profiles of decreasing conductivity with depth. It is worth noting that increasing the amplitude of the noise

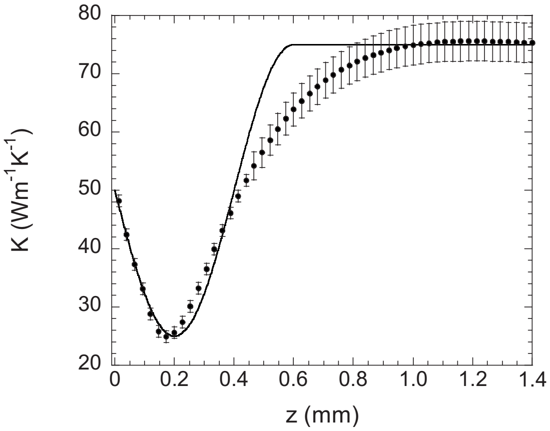

FIG. 2. Real (line) and reconstructed (symbols) oscillating conductivity profile obtained from calculated data with added white noise similar to our experimental noise. The dots represent the mean value of the conductivity retrieved at each depth from a linear initial guesses (25 W/mK at the surface and 50 W/mK in bulk), and different noise vectors and bulk conductivity depths.

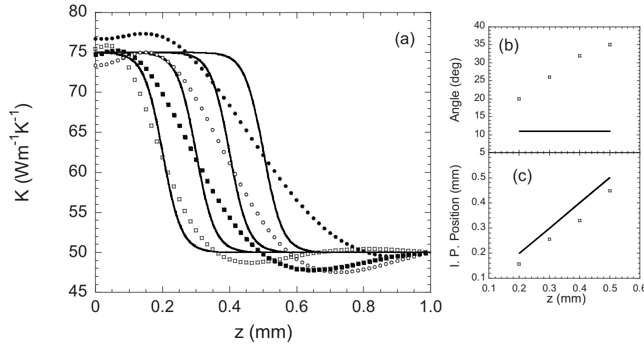

FIG. 3. (a) Real (lines) and retrieved (symbols) sigmoidal conductivity profiles obtained from calculated data with added white noise similar to our experimental noise. The inflexion points of the real profiles are located at 0.2, 0.3, 0.4, and 0.5 mm beneath the surface. The symbols represent single reconstructions obtained with flat initial conductivity (50 $\mathrm{Wm^{-1}\,K^{-1}}$) and bulk conductivity at 1 mm. (b) Angle of the reconstructed (symbols) and true (line) profiles with the vertical at the position of the inflexion point, as a function of the position of the inflexion point of the real profiles, (c) position of the inflexion point for reconstructed (symbols) and real (line) profiles, as a function of the position of the inflexion point (of the real profiles).

vectors does not significantly affect the retrieved profiles, indicating that the Tikhonov regularization procedure is very well suited for the reconstruction of exponential profiles. This is also the reason why the initial value of the regularization parameter is not very relevant to reach convergence.

B. Oscillating profiles

Similar calculations have been performed in the case of a conductivity showing an oscillating behavior, like the solid line shown in Fig. 2. In this case, it is worth mentioning the relationship between the choice of the initial guess and the value of the initial regularization parameter. Their influence in oscillating profiles is much more pronounced than in exponentials. We have checked that, unless the initial regularization parameter is sufficiently high, convergence cannot be reached. Of course, the best choice of the initial regularization parameter is the lowest possible, since higher values lead to long iteration processes. For an initial guess consisting in a linearly increasing conductivity, from 25 $\mathrm{Wm^{-1}\,K^{-1}}$ at the surface to 50 $\mathrm{Wm^{-1}\,K^{-1}}$ in bulk, an initial regularization parameter of $100\alpha_0$ was high enough. However, if we start from a flat (50 $\mathrm{Wm^{-1}\,K^{-1}}$) or decreasing (75 $\mathrm{Wm^{-1}\,K^{-1}}$ at the surface to 50 $\mathrm{Wm^{-1}\,K^{-1}}$ in bulk) conductivity profiles, the initial regularization parameter must be increased by two orders of magnitude in order to reach convergence. The reason for this is that, for an initial guess very different from the true profile, the first iterations of the reconstruction might bring the system to meaningless negative conductivities. However, increasing the size of the initial penalization enlarges the convergence domain, i.e., it increases the possible choices of the initial guess leading to the global minimum. This shows that the method is able to bring the system to convergence when it is forced with a not so realistic initial guess.

Regarding the order of the Tikhonov functionals, we have found that zero order Tikhonov regularization leads to reconstructed conductivities with oscillating artifacts. For this reason, we have performed all the inversions using first order Tikhonov regularization. As an example of oscillating profile, in Fig. 2 we show a pipelike K profile together with its reconstruction. In this case the initial guess is an increasing linear profile with 25 $\mathrm{Wm^{-1}\,K^{-1}}$ conductivity at the surface and 50 $\mathrm{Wm^{-1}\,K^{-1}}$ conductivity in bulk, and the initial regularization parameter is $100\alpha_0$. As can be seen in the figure, the reconstruction is quite good at positions close to the surface but there is a significant discrepancy between the true and reconstructed conductivities in depth. Actually, the reconstructed profile is much smoother than the real one, meaning that the steep behavior close to the bulk is barely reproducible.

C. Sigmoidal profiles

Very often, the thermal conductivity profiles of heterogeneous samples, as is the case of hardened steels and cured dental resins, show quasisigmoidal shapes.[3,4,16] For this reason, it is especially interesting to analyze the accuracy of the Tikhonov method to retrieve this kind of profiles. We have retrieved sigmoidal conductivity profiles with different slopes and located at different depths, both with increasing and decreasing conductivity with depth. Again, in all cases, the zero order Tikhonov functional leads to more artificially oscillating reconstructions than the first order functional, so we will only show profiles obtained using the first order functional.

In Fig. 3(a) we show single reconstructions of sigmoidal decreasing conductivity profiles all with the same (steep) slope but located at different depths. All the calculations were performed by inverting synthetic amplitude and phase data corresponding to the profiles shown in solid lines with added white noise similar to the experimental noise. As can be seen, for this steep function, the reconstructed conductivities underestimate the slopes of the profiles, the differences between real and reconstructed slopes being larger as the depth of the "step" increases. In order to quantify the quality of the reconstruction, we have first compared the angle of the curves with the vertical at the position of the inflexion point [Fig. 3(b)] for both, reconstructed (symbols) and real (line) profiles, as a function of the depth of the inflexion point. It can be observed that the angle is dramatically underestimated, especially as the depth of the inflexion point increases. Then, we have compared the position of the inflexion point [Fig. 3(c)] for both, reconstructed (symbols) and real (line) profiles, as a function of the position of the inflexion point of the real profiles. As can be seen, unlike the angle, the position of the inflexion point is quite well reproduced, although slightly underestimated. This indicates that, despite the severe underestimation of the slope, the method quite accurately determines the position of the inflexion point, which can be used to roughly locate the case penetration depth.

We have reduced the white noise added to the synthetic data in order to evaluate its influence on the retrieved angle and inflexion point. We have found that, in the worse conditions we have studied, i.e., for a real sigmoidal profile with its inflexion point located 0.5 mm beneath the surface and with a slope like the one shown Fig. 3(a), the noise needs to be reduced down to three orders of magnitude in order to retrieve the right angle. Two consequences can be derived from this result: first, in a real case the Tikhonov regularization does not give optimum results when the sigmoidal profile is steep. Second, the method converges to the exact result when the noise is reduced, which is a desirable property of an inversion procedure.

In Fig. 4 we show, in circles, the reconstructed conductivities corresponding to three real increasing conductivity profiles (lines). In Figs. 4(a) and 4(b) we show profiles with the same (steep) slope but with their inflexion points located at 0.2 mm and 0.5 mm beneath the surface, respectively, and in Fig. 4(c) we show a smoother slope, with its inflexion point located 0.5 mm beneath the surface. All these reconstructions were performed using first order Tikhonov regularization term. The tests performed in order to determine the optimum initial regularization parameter gave similar results as in the case of the oscillating profile: for values smaller than $100\alpha_0$, no convergence could be reached so $100\alpha_0$ was found to be the best initial regularization parameter. As can be observed, if we look at the mean conductivities [rather than at single reconstructions as in Fig. 3(a)] we also observe that for the steep slopes depicted in Figs. 4(a) and 4(b), the deeper the transition, the bigger the underestimation of the slope. Moreover, in these increasing profiles the mean conductivities retain the spurious oscillations in flat regions that we observed in the single reconstructions of decreasing profiles. However, the result of calculating the mean conductivity attenuates the oscillations but increases the error bar in flat (real) regions. If we compare Figs. 4(b) and 4(c), representing two profiles with their inflexion points located at the same position but with different slopes, it is quite evident that the reconstruction of the smoother profile is more accurate. As illustrated in this figure, the method is more suitable to reconstruct smooth than steep profiles. We would like to emphasize that, even when using the first order Tikhonov function, all the reconstructed profiles still exhibit some spurious oscillations in the (real) flat regions, an artifact that we cannot avoid with this method. All these results indicate that, in general the reconstructed sigmoidal conductivity profiles using the Tikhonov regularization procedure underestimate the slopes of the profiles.

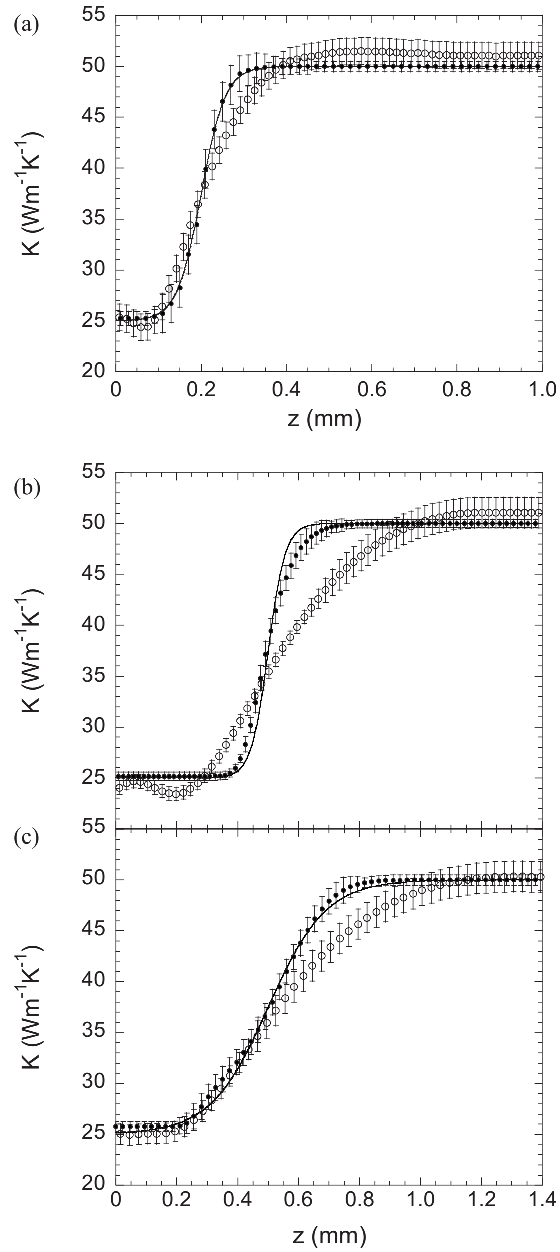

FIG. 4. Real (lines) and reconstructed (symbols) sigmoidal conductivity profiles retrieved by using the Tikhonov regularization (circles) and the TV regularization (dots), obtained from calculated data with added white noise similar to our experimental noise. The symbols represent the mean value of the conductivity retrieved at each depth from different initial guesses, (a) steep profile, with inflexion point located at 0.2 mm, (b) steep profile, with inflexion point located at 0.5 mm, and (c) smooth profile, with inflexion point located at 0.5 mm

Once the Tikhonov regularization has proven to give oversmoothed sigmoidal conductivity reconstructions, the question is now how to proceed in a real case, where the true conductivity is unknown. A first hint that the Tikhonov function is not working fully properly is the appearance of the oscillations mentioned above. The method is not suitable to reproduce the flat sections in sigmoidal profiles. Actually, other regularization functionals are much better suited to reconstruct profiles with sparse flat sections, like the total variation (TV) regularization[21]

$$TV(K_1, \ldots, K_N, K_{\text{unhardened}}) = \sum_{j=1}^{N-1} |K_{j+1} - K_j| + |K_{\text{unhardened}} - K_N|, \tag{5}$$

where we have added a Dirichlet boundary condition on the deepest layer. If compared to the first order Tikhonov functional [Eq. (4)], it could be described as a functional with a pre-established flat initial guess. Moreover, since the addends correspond to the absolute values of the differences between the conductivities of adjacent layers, the functional represents the "TV" of the conductivity profile. According to the previous discussion, in cases where the Tikhonov regularization gives quasisigmoidal, oscillating reconstructions, we propose to perform an alternative minimization by using a regularization TV functional, in the following way: as the TV functional is not linear, for each linearization of the discrepancy term we approximate the TV functional by means of fix point iterations that lead to quadratic regularization terms as the following:

$$TV^* = \sum_{j=1}^{N-1} \frac{(K_{j+1} - K_j)^2}{\varepsilon + |K^*_{j+1} - K^*_j|} + \frac{(K_{\text{unhardened}} - K_N)^2}{\varepsilon + |K_{\text{unhardened}} - K^*_N|}, \tag{6}$$

where ε is a small constant (10^{-5} for instance) added to avoid divergence in sparse blocks and the asterisk in the denominator represents the conductivities corresponding to previous fix point iteration. This is the reason why this approximation can be interpreted as a weighted/lagged Tikhonov functional. Note that, when the conductivities retrieved in successive fix point iterations are not very different from each other, this term is a good approximation of the TV regularization.

We have checked the TV regularization for the three real sigmoidal profiles represented in lines in Fig. 4. The corresponding results are depicted in dots in Fig. 4: in all three cases the oscillations disappear and the slope of the reconstructed profile is much closer to the slope of the real profile, meaning that the reconstructions using the TV functional is more accurate than the reconstruction with Tikhonov functional for this kind of profiles. The reason for such different reconstructions when using the Tikhonov and TV regularization is the following: when a penalty is introduced to stabilize the minimization the penalty term restricts the kind of functions the search will be made through. In the case of the first order Tikhonov functional, steplike functions (having infinite slope) are avoided since they lead the penalty term to diverge, so the search is performed among smooth functions, as stated before. On the contrary, the TV regularization searches through functions whose TV is finite, [bounded variation (BV) functions] without restrictions on the values of their derivatives; steplike functions are among BV functions and have zero slope in the flat regions, as the "associated" initial guess, so steepest reconstructions are retrieved with this regularization. Note also that the error bars corresponding to the TV reconstructions are wider in the region where the conductivity is changing than in the flat regions.

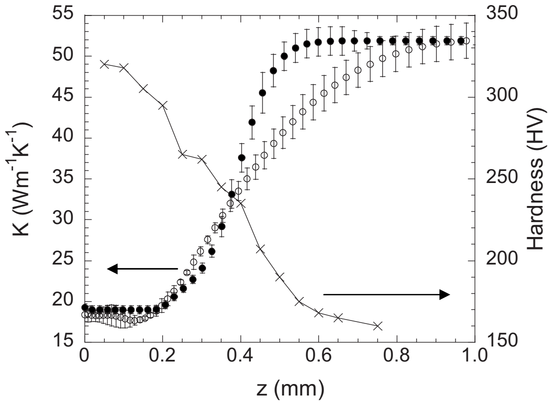

FIG. 5. Results of the indentation test (crosses) correspond to the experimental data of Ref. 4, together with the reconstructed conductivity profiles using the Tikhonov regularization (circles) and the TV regularization (dots). The continuous line is a guide for the eye.

The reason for this is that, since the method searches among steplike functions, small variations in the location of the step lead to a big uncertainty in the value of the conductivity. As in the reconstructions we are performing we let the position of the unhardened material to be located at different depths, the final reconstruction (the mean of all reconstructions performed) is smoother than the individual reconstructions and exhibits a larger uncertainty in the region close to the inflexion point.

All the discussion above leads us to revisit the results obtained previously with real data. After the previous analysis we can conclude that the reconstructed profile shown in Fig. 5 of Ref. 4, corresponding to a case hardened AISI 1018 steel plate, is very likely smoother than the real one. This is in agreement with the results of microindentation tests performed in the same sample,[22] showing a steeper profile. Accordingly, we have applied this TV regularization to the inversion of the experimental data. In Fig. 5 we present the microindentation results together with the reconstructions using the Tikhonov regularization and the TV regularization. As can be observed, the reconstruction using Tikhonov is smoother than the microindentation profile, and the one using TV is closer to the microindentation test, although slightly steeper. Even if this last reconstruction does not fully reproduce the shape of the microindentation test, it certainly represents an improvement with respect to the results of previous methods used to reconstruct case hardening conductivity profiles. Finally we would like to stress that the method we have presented assumes random errors in experimental data and also deals with of systematic errors in the case they result in a factor affecting the amplitudes and a shift in the phase. However, the presence of other systematic errors is the main difficulty in the application of these methods to real problems, and leads to excessively optimistic assumed accuracy of the reconstructions. For instance, the presence of three-dimensional heat propagation due to lateral diffusion (at low frequencies) can significantly alter the surface temperature amplitude and phase in such a way that reconstructions obtained by working with a ID model can be completely distorted.[23]

IV. CONCLUSIONS

We have analyzed the suitability of the Tikhonov regularization method to reconstruct thermal conductivity depth-profiles with shapes similar to those found in real heterogeneous sample, as is the case of hardened steels and cured dental resins. We have analyzed the influence of the order of the Tikhonov function, of the initial value of the regularization parameter, of the initial guess, and of the experimental noise on the final reconstruction. From this study we can conclude that this type of regularization gives very good results when the profile to be reconstructed is smooth, like exponential profiles, but it fails when the profile is steep, especially if the step is located deep inside the material. Moreover, we have observed spurious oscillations appearing in the reconstructed conductivities, corresponding to regions of flat conductivity on the real profiles, indicating that the Tikhonov regularization is not the optimum choice in these cases. We have studied the TV regularization as a natural alternative when the reconstructed conductivity presents quasiflat oscillating regions. The application of TV regularization in these cases gives much better results than Tikhonov regularization. According to the results we propose the following procedure for a real case, where the conductivity is unknown: perform the inversion using the Tikhonov regularization, check for oscillating behaviors both close to the surface and deep inside the material and, if oscillations occur, perform a second inversion by regularizing with a TV functional. Unlike other methods, only minor *a priori* information about the conductivity profile is used in order to improve the fidelity of the reconstructed profiles, namely: the noise level of the experimental data, the conductivity of the unhardened material and an assumption about nuances of the conductivity profile: smoothness which makes us choose the Tikhonov regularization first, and lack of oscillations, in shallow and deep locations, which brings us to try TV regularization. The application of this method to real experimental data of a case hardened steel plate has given a very good quantitative anticorrelation with the indentation test results. We expect that the development of this method will contribute to increase the reliability of local inversion methods.

ACKNOWLEDGMENTS

This work has been supported by the Ministerio de Educación y Ciencia through research Grant No. MAT2008-01454, by the Universidad del País Vasco through research Grant No. DIPE08/10, and by the Diputación General de Aragón.

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