

On determination of the relaxation spectrum of viscoelastic materials from discrete-time stress relaxation data

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Summary. The paper deals with the problem of recovery of continuous relaxation spectrum of linear viscoelastic materials from discrete-time noise corrupted measurements of relaxation modulus obtained in stress relaxation test. The least-squares problem of optimal approximation of the spectrum is solved based on the orthogonal series expansion. Hermite functions are used. Since the problem of relaxation spectrum identification is ill-posed, the inverse problem of Tikhonov regularization is used to guarantee the stability of the scheme. Guaranteed model approximation (GMA) is adopted for the choice of the regularization parameter. The numerical realization of the scheme by using the singular value decomposition (SVD) is discussed. The resulting identification algorithm is described in forthcoming paper.

Key words: viscoelasticity, relaxation spectrum, identification, regularization, Hermite functions

INTRODUCTION

Many materials are most often modelled in a time-domain viscoelastic regime, which is good for characterizing strain-stress dependence, creep and stress relaxation within a small deformation [1, 2, 4, 5, 7, 15, 16]. Although for viscoelastic materials a multiplicity of constitutive theories exists, essentially, only linear viscoelasticity is considered for which the Boltzmann superposition principle applies.

The mechanical properties of linear viscoelastic materials are characterized by relaxation spectrum [4, 5, 13, 16]. From the relaxation spectrum other material functions such as the relaxation modulus or the creep compliance can be calculated without difficulty and next both the constant and time-variable bulk and shear modulus or Poisson's ratio can be determined. Thus, the spectrum is vital not only for constitutive models but also for the insight into the properties of a viscoelastic material [13,19,27].

Relaxation spectrum is not directly accessible by experiment and thus must be determined from the appropriate response function, measured either in time or frequency domain [4, 13, 15, 27]. There are a few papers, e.g., [27] as well as [18-20] and the other previous papers by the present author cited therein, that deal with the relaxation spectrum determination from time-measurement data. However, the computationally efficient methods to determine the spectrum are still desirable and it is the purpose of this study.

The practical difficulty in the relaxation spectrum determination is rooted in a theoretical mathematical problem difficulty, because it is an ill-posed inverse problem [4,19]. The mathematical difficulties can be overcome by synthesis of an appropriate identification algorithm. In this paper an optimal scheme of the least-squares approximation of relaxation spectrum by the linear combination of Hermite functions is proposed. The assumed quality of the model approximation is achieved by the respective choice of the regularization parameter by using guaranteed model approximation rule.

RELAXATION SPECTRUM

In the rheological literature it is commonly assumed that the modulus $G(t)$ has the following relaxation spectrum representation [5,16]:

$$G(t) = \int_0^{\infty} H(\nu) e^{-t\nu} d\nu, \quad (1)$$

where: the relaxation spectrum $H(\nu)$ characterizes the distribution of relaxation frequencies $\nu \geq 0$ in the range $[\nu, \nu+d\nu]$. We assume that the real relaxation spectrum $H(\nu)$ there exists – the respective existence and uniqueness conditions are given in [21; Part I: Theorem 1, Part II: Theorems 1, 2]. Throughout we shall be concerned with

the case when the spectrum $H(\nu)$ is completely unknown; the relaxation modulus $G(t)$ can be, however, measured for any time $t \geq 0$.

The problem of relaxation spectrum determination is the numerical problem of reconstructing solution of Fredholm integral equation of the first kind (1) from time-measured discrete relaxation modulus data. This problem is known by Hadamard to be severely ill-posed [19, 23]. This means that small changes in measurement data can lead to arbitrarily large changes in the relaxation spectrum. In remedy, some reduction of the admissible solutions set or respective regularization of the original problem can be used. In this paper we use both the techniques simultaneously. An approximation of the spectrum by the finite series of Hermite functions is combined with Tikhonov regularization.

The idea of the scheme is based on the Fourier series expansion of unknown relaxation spectrum with respect to the orthonormal basis in function space. This approach is known both in the approximation theory [25] and in mathematical modelling and system identification tasks [8,9,14]. A wide overview of the significance of the orthogonal basis in system identification is available in [14]. Orthogonal schemes are also used for signal processing [9] and in automatic control algorithms [3,26]. In the identification of mathematical models of viscoelastic material orthogonal series expansion approach is used both for linear materials, e.g., [15,19,20], and for nonlinear materials for example in [3]. The Hermite polynomials are applied for systems identification, for example in [6].

MODELS

Assume that $H(\nu) \in L_2(0, \infty)$, where $L_2(0, \infty)$ is the space of square-integrable functions on the interval $(0, \infty)$. The respective sufficient conditions are given in [21; Part II: Theorem 3]. Let $h_k(\nu)$, $k=0,1,\dots$; let the Hermite functions be given by [12]:

$$h_k(\nu) = \frac{\sqrt{\alpha}}{\sqrt{2^k k! \sqrt[4]{\pi}}} e^{-(\alpha\nu)^2/2} P_k(\alpha\nu), \quad k = 0, 1, \dots, \quad (2)$$

where: $P_k(x)$ is Hermite polynomial of degree k defined by recursive formula [12]:

$$P_k(x) = 2xP_{k-1}(x) - 2(k-1)P_{k-2}(x), \quad k = 2, 3, \dots, \quad (3)$$

starting with:

$$P_0(x) = 1 \text{ and } P_1(x) = 2x, \quad (4)$$

where: $\alpha > 0$ is a time-scaling factor.

We assume that the model of the relaxation spectrum is to be selected within the parametric class of models defined by the finite sum:

$$H_K(\nu) = \sum_{k=0}^{K-1} g_k h_k(\nu), \quad (5)$$

where: g_k are constant model parameters, the lower index of $H_K(\nu)$ is the number of model summands. Then, the respective model of the relaxation modulus is described by:

$$G_K(t) = \int_0^\infty H_K(\nu) e^{-t\nu} d\nu = \sum_{k=0}^{K-1} g_k \phi_k(t), \quad (6)$$

where, according to equation (1), the functions $\phi_k(t)$ are defined as:

$$\phi_k(t) = \int_0^\infty h_k(\nu) e^{-t\nu} d\nu. \quad (7)$$

The useful recursive form of the basis functions $\phi_k(t)$ is given by the following theorem; the proof, as well as the proofs of the next results, is omitted due to space limitations.

Theorem 1. Let $\alpha > 0$ and $t \geq 0$. Then the basis functions $\phi_k(t)$ (7) are given by the recursive formula:

$$\begin{aligned} \phi_{k+1}(t) = & \frac{1}{\sqrt{2^{k-1} \alpha (k+1)! \sqrt[4]{\pi}}} P_k(0) - \\ & - \frac{\sqrt{2}}{\alpha \sqrt{k+1}} t \phi_k(t) + \frac{\sqrt{k}}{\sqrt{k+1}} \phi_{k-1}(t), \quad k \geq 1, \end{aligned} \quad (8)$$

starting with:

$$\phi_0(t) = \frac{\sqrt[4]{\pi}}{\sqrt{2\alpha}} e^{-t^2/(2\alpha^2)} \operatorname{erfc}(t/(\sqrt{2}\alpha)), \quad (9)$$

$$\phi_1(t) = \frac{\sqrt{2}}{\sqrt{\alpha} \sqrt[4]{\pi}} - \frac{\sqrt{2}}{\alpha} t \phi_0(t), \quad (10)$$

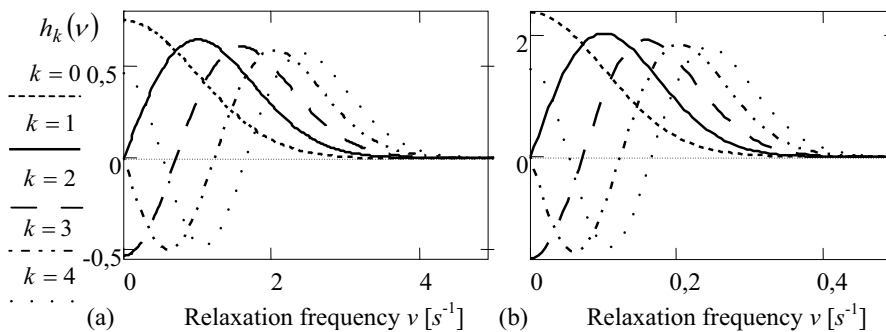


Fig. 1. The Hermite basis functions $h_k(\nu)$ for parameters: (a) $\alpha = 1[s]$ and (b) $\alpha = 10[s]$; $k=0,1,2,3,4$

where the function:

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt, \quad x \geq 0, \quad (11)$$

is complementary error function [12].

The values $P_k(0)$ of Hermite polynomials are given by:

$$P_{2k}(0) = (-1)^k (2k)!/k! \text{ and } P_{2k+1}(0) = 0. \quad (12)$$

A few first basis functions $h_k(v)$ are shown in Figure 1 for two different values of the time-scaling factor α ; the corresponding functions $\phi_k(t)$ are plotted in Figure 2.

Note that from Figure 2 it is evident that the basis functions are congruent to the real relaxation modulus obtained in experiment. The parameter $\alpha > 0$ is the time-scaling factor. The following rule holds: the lower the parameter α is, the shorter the relaxation times are, i.e. the greater are the relaxation frequencies. The above is illustrated by Figures 1 and 2. What must be done to salvage it is to find some way of determining the basis functions which ‘look like’ the real relaxation modulus. To further this end, we must choose the respective time scale factor α .

AUGMENTED MODEL

It is well-known [5,16,19] that for many materials $\lim_{t \rightarrow \infty} G(t) = G_{\infty} > 0$, where G_{∞} is the long-term modulus. It is also the case of the beet root sample, which is considered in [22; Example 3]. Thus, instead of the classical model (6), it is convenient to consider the following augmented model:

$$\bar{G}_K(t) = \int_0^{\infty} H_K(v) e^{-tv} dv + G_{\infty} = G_K(t) + G_{\infty}. \quad (13)$$

Then, the relaxation spectrum model takes the form:

$$\bar{H}_K(v) = H_K(v) + G_{\infty} \delta(v), \quad (14)$$

where: $H_K(v)$ is given by (5) and $\delta(v)$ denotes the Dirac delta function. Unbounded component $G_{\infty} \delta(v)$ of the relaxation spectrum $\bar{H}_K(v)$ (14) corresponds with the relaxation frequency equal to zero, or equivalently, with infinite relaxation time.

IDENTIFICATION PROBLEM

Classical manner of studying viscoelasticity is by two-phase stress relaxation test, where the time-dependent shear stress is studied for step increase in strain [16, 24]. In the first initial phase the strain should be imposed instantaneously. During the second phase the corresponding force induced in the specimen, which decreases with time, is measured.

Suppose a stress relaxation test performed on the specimen of the material under investigation resulted in a set of measurements of the modulus $\bar{G}(t_i) = G(t_i) + z(t_i)$ at the sampling instants $t_i \geq 0, i = 1, \dots, N$, where $z(t)$ is measurement noise.

Identification consists of selection within the given class of models defined by (6), (13) of such a model, which ensures the best fit to the measurement results. As a measure of the model (6), (13) accuracy the square index commonly used in identification theory [6, 10, 19, 20] and experimental studies [11, 19, 20] is taken:

$$Q_N(\mathbf{g}_K) = \sum_{i=1}^N [\bar{G}(t_i) - \bar{G}_K(t_i)]^2 = \|\bar{\mathbf{G}}_N - \Phi_{N,K} \mathbf{g}_K\|_2^2, \quad (15)$$

where: $\|\cdot\|_2$ denotes the square norm in the Euclidean space, $\mathbf{g}_K = [g_0 \dots g_{K-1} G_{\infty}]$ is an $(K+1)$ – element vector of unknown coefficients of the model (6), (13). The $N \times (K+1)$ – element matrix $\Phi_{N,K}$ and the vector $\bar{\mathbf{G}}_N$ are defined as:

$$\Phi_{N,K} = \begin{bmatrix} \phi_0(t_1) & \dots & \phi_{K-1}(t_1) & 1 \\ \vdots & \ddots & \vdots & \vdots \\ \phi_0(t_N) & \dots & \phi_{K-1}(t_N) & 1 \end{bmatrix}, \quad \bar{\mathbf{G}}_N = \begin{bmatrix} \bar{G}(t_1) \\ \vdots \\ \bar{G}(t_N) \end{bmatrix}. \quad (16)$$

Thus, the optimal identification of relaxation spectrum in the class of functions $\bar{H}_K(v)$ given by (5), (14) consists of solving, with respect to the model parameter \mathbf{g}_K , the least-squares problem with the index (15). The matrix $\Phi_{N,K}$ is usually ill-conditioned. Then, the minimum of (15) is not unique and even the normal (minimum Euclidean norm) solution of the linear-quadratic problem (15)-(16) is non-continuous and unbounded function of the data vector $\bar{\mathbf{G}}_N$, i.e. when the data are noisy even small changes in $\bar{\mathbf{G}}_N$ would lead to arbitrarily large artefact in $\bar{\mathbf{g}}_K^N$. This is a crucial point of the problem. To deal with the ill-posedness, the Tikhonov regularization method is used as presented in the subsequent section.

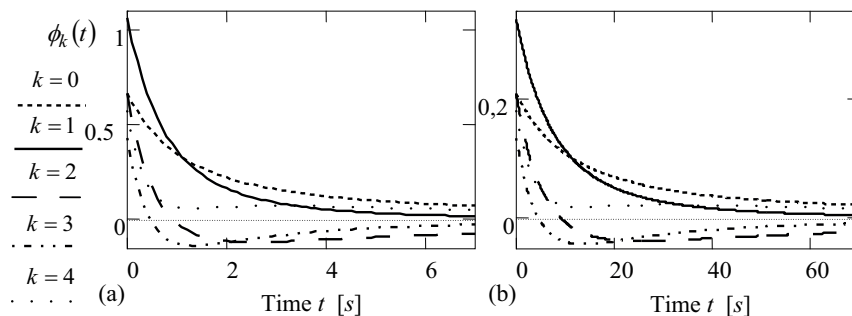


Fig. 2. Functions $\phi_k(t)$ of Hermite algorithm, the parameters: (a) $\alpha = 1[s]$ and (b) $\alpha = 10[s]$; $k = 0, 1, 2, 3, 4$

REGULARIZATION

Tikhonov regularization [23] strives to stabilize the computation of the least-squares solution by minimizing a modified square functional of the form:

$$\min_{\mathbf{g}_K \in R^K} \left\| \bar{\mathbf{G}}_N - \Phi_{N,K} \mathbf{g}_K \right\|_2^2 + \lambda \left\| \mathbf{g}_K \right\|_2^2, \quad (17)$$

where: $\lambda > 0$ is a regularization parameter. The above problem is well-posed, that is the solution always exists, is unique, and continuously depends on both the matrix $\Phi_{N,K}$ as well as on the measurement data $\bar{\mathbf{G}}_N$. The model parameter vector minimizing (17) is given by:

$$\mathbf{g}_K^\lambda = \left(\Phi_{N,K}^T \Phi_{N,K} + \lambda \mathbf{I}_{K+1,K+1} \right)^{-1} \Phi_{N,K}^T \bar{\mathbf{G}}_N, \quad (18)$$

where: $\mathbf{I}_{K+1,K+1}$ is $(K+1) \times (K+1)$ identity matrix.

The choice of regularization parameter λ is crucial to identify the best model parameters. Here we apply the guaranteed model approximation (GMA) rule, which is presented in details below. The choice of the regularization parameter according to GMA does not depend on *a priori* knowledge about the noise variance.

ALGEBRAIC BACKGROUND

For numerical computation of regularized solution (18), the singular value decomposition (SVD) technique will be used. Let SVD of the matrix of the matrix $\Phi_{N,K}$ take the form [17]:

$$\Phi_{N,K} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T, \quad (19)$$

where: $\mathbf{V} \in R^{K+1,K+1}$ and $\mathbf{U} \in R^{N,N}$ are orthogonal matrices and $\mathbf{\Sigma} = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0)$ is $N \times (K+1)$ diagonal matrix containing the non-zero singular values $\sigma_1, \dots, \sigma_r$ of the matrix $\Phi_{N,K}$ with $r = \text{rank}(\Phi_{N,K})$ [17]. Taking advantage of the diagonal structure of $\mathbf{\Sigma}$ and the matrices \mathbf{V} and \mathbf{U} orthogonality, it may be simply proved that [19]:

$$\mathbf{g}_K^\lambda = \mathbf{V} \mathbf{A}_\lambda \mathbf{U}^T \bar{\mathbf{G}}_N, \quad (20)$$

where: the diagonal structure matrix \mathbf{A}_λ is as follows:

$$\mathbf{A}_\lambda = \text{diag} \left(\sigma_1 / (\sigma_1^2 + \lambda), \dots, \sigma_r / (\sigma_r^2 + \lambda), 0, \dots, 0 \right). \quad (21)$$

GUARANTEED MODEL APPROXIMATION

We wish to introduce a simple rule for the choice of the regularization parameter, in which the value of the identification index is directly taken into account. It may be proved that for an arbitrary $\lambda > 0$ the following equality holds:

$$Q_N \left(\mathbf{g}_K^\lambda \right) = \sum_{i=1}^r \frac{\lambda^2 y_i^2}{(\sigma_i^2 + \lambda)^2} + Q_N \left(\bar{\mathbf{g}}_K^N \right), \quad (22)$$

where: $\bar{\mathbf{g}}_K^N$ of the normal solution of the least-squares task (15)-(16) for noise-free data $\mathbf{G}_N = [G(t_1) \dots G(t_N)]$ and y_i are the elements of the vector $\mathbf{Y} = \mathbf{U}^T \bar{\mathbf{G}}_N$. Hence $Q_N \left(\mathbf{g}_K^\lambda \right) > Q_N \left(\bar{\mathbf{g}}_K^N \right)$. The deterioration of the model quality is a result of the stabilization of the linear least-squares task (15). However, the assessment of model quality is typically based on how the model performs when it attempts to reproduce the measured data. This is the viewpoint we are going to adopt. Focusing then more on the model quality in this section we shall introduce the guaranteed model approximation (GMA) rule of the choice of the regularization parameter. Some of its properties will also be demonstrated. The idea behind GMA rule is to choose the regularization parameter so that the assumed quality of the model approximation index $\hat{Q}_N > Q_N \left(\bar{\mathbf{g}}_K^N \right)$ is achieved, i.e., such a parameter $\hat{\lambda}$ for which $Q_N \left(\mathbf{g}_K^{\hat{\lambda}} \right) = \hat{Q}_N$. Appealing to the equation (22) this rule consists in solving - with respect to λ - of the following equation:

$$\sum_{i=1}^r \frac{\lambda^2 y_i^2}{(\sigma_i^2 + \lambda)^2} + Q_N \left(\bar{\mathbf{g}}_K^N \right) = \hat{Q}_N, \quad (23)$$

where: $Q_N \left(\bar{\mathbf{g}}_K^N \right) = \sum_{i=r+1}^N y_i^2$. The GMA rule was at first applied for the relaxation times spectrum identification in early authors' work [18]. This rule seems to be quite a natural strategy in the context of relaxation spectrum identification task in which the identification index refers to the relaxation modulus approximation quality. Note that if there exists an $1 \leq i \leq r$ such that $y_i \neq 0$, then the quality index $Q_N \left(\mathbf{g}_K^\lambda \right)$ is monotonically increasing function of $\lambda > 0$ (compare eq. (22)). Thus, the equation (23) has a unique solution $\hat{\lambda} > 0$ whenever $\hat{Q}_N > Q_N \left(\bar{\mathbf{g}}_K^N \right)$ and there exists $y_i \neq 0, 1 \leq i \leq r$. Simple *a posteriori* criteria for when the last condition is satisfied are given by the following corollary proved in [19; Property C.1].

Corollary. Let $K \geq 1, r = \text{rank}(\Phi_{N,K}) < N$ and $N \geq K$. If so, there exists an $1 \leq i \leq r$ such that $y_i \neq 0$ if and only if $\Phi_{N,K}^T \bar{\mathbf{G}}_N \neq \mathbf{0}_{K+1}$, where $\mathbf{0}_{K+1}$ denotes $(K+1)$ -vector of zero elements.

Thus, we now have a more convenient way of characterizing when the solution of GMA rule exists, since the SVD decomposition of the matrix $\Phi_{N,K}$ is not required here.

Both the function:

$$F(\lambda, \mathbf{\Sigma}, \mathbf{Y}) = \sum_{i=1}^r \frac{\lambda^2 y_i^2}{(\sigma_i^2 + \lambda)^2} + Q_N \left(\bar{\mathbf{g}}_K^N \right) - \hat{Q}_N, \quad (24)$$

and the derivative:

$$F'_\lambda(\lambda, \mathbf{\Sigma}, \mathbf{Y}) = 2\lambda \sum_{i=1}^r \frac{y_i^2 \sigma_i^2}{(\sigma_i^2 + \lambda)^3}, \quad (25)$$

can be expressed by convenient formulas as functions of singular values $\sigma_1, \dots, \sigma_r$ and elements y_i of the vector \mathbf{Y} . Thus, in order to find a solution $\hat{\lambda}$ of equation (23), i.e. $F(\hat{\lambda}, \mathbf{\Sigma}, \mathbf{Y}) = 0$, the Newton scheme can be successfully applied, in which the successive approximation of the regularization parameter $\hat{\lambda}$ is computed according to the formula:

$$\lambda_{n+1} = \lambda_n - \frac{F(\lambda_n, \mathbf{\Sigma}, \mathbf{Y})}{F'_{\lambda}(\lambda_n, \mathbf{\Sigma}, \mathbf{Y})}.$$

An arbitrary $\lambda_0 \neq 0$ can be taken as an initial point. The functions $F(\lambda, \mathbf{\Sigma}, \mathbf{Y})$ (24) and $F'_{\lambda}(\lambda, \mathbf{\Sigma}, \mathbf{Y})$ (25) depend continuously on every argument. Thus, on the basis of the well-known implicit function theorem the solution $\lambda = \hat{\lambda}(\mathbf{\Sigma}, \mathbf{Y})$ is continued with respect to the matrix $\mathbf{\Sigma}$ and vector \mathbf{Y} . Thus, the above GMA rule is well-posed in the Hadamard sense.

A certain interpretation of the GMA rule and important property of the solution:

$$\hat{\mathbf{g}}_K = \mathbf{g}_K^{\hat{\lambda}} \quad (26)$$

are given in the following result. The conclusion follows immediately from a quick inspection of the proof of [18; theorem 2].

Theorem 2. Assume $K \geq 1$, $N \geq K$ and $\hat{Q}_N > Q_N(\bar{\mathbf{g}}_K^N)$. The regularized solution $\hat{\mathbf{g}}_K$ defined by (23) and (26) is the unique solution of the following optimization task:

$$\min_{\mathbf{g}_K \in R^K} \|\mathbf{g}_K\|_2^2 \text{ under the constraint } Q_N(\mathbf{g}_K^{\lambda}) \leq \hat{Q}_N.$$

By theorem 2 the GMA rule (23) relies in such a selection of the relaxation spectrum model that the norm of the vector $\hat{\mathbf{g}}_K$ (26) has the smallest possible value among all models such that $Q_N(\mathbf{g}_K) \leq \hat{Q}_N$. Thus the best smoothness of the model parameters vector $\hat{\mathbf{g}}_K$ (26) is achieved. The effectiveness of this approach in the context of relaxation spectrum identification has been verified by the earlier authors' works, see [18, 19].

CONCLUSIONS

The problem of the relaxation spectrum calculation from discrete-time linear relaxation modulus noise data is solved based on the least-squares approximation of the spectrum by finite linear combination of the basic Hermite functions. As a result, the primary infinite dimensional dynamic optimization problem of the continuous relaxation spectrum identification is reduced to the static linear-quadratic programming task. Tikhonov regularization and guaranteed model approximation are used to solve it. The analysis of the scheme stability, noise robustness, smoothness and convergence as well as simulation tests using both artificial and experimental data are the subject of the next paper [22].

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O IDENTYFIKACJI SPECTRUM RELAKSACJI
MATERIAŁÓW LEPKOSPĘŻYSTYCH NA PODSTAWIE
DYSKRETNÝCH POMIARÓW MODUŁU RELAKSACJI

Streszczenie. Praca dotyczy problemu wyznaczenia ciągłego spektrum relaksacji materiałów o własnościach liniowo-lepkospężytych na podstawie dyskretnych zakłóconych pomiarów modułu relaksacji uzyskanych w teście relaksacji naprężeń. Problem rozwiązano przybliżając spektrum relaksacji skończonym szeregiem funkcji Hermita optymalnie w sensie zregulowanej metody najmniejszej sumy kwadratów. Zastosowano regularyzację Tichonowa. Współczynnik regularyzacji dobrano metodą gwarantowanej jakości modelu (ang. guaranteed model approximation). Odpowiedni algorytm identyfikacji będzie przedmiotem następnej pracy.

Słowa kluczowe: lepkospężytość, spectrum relaksacji, identyfikacja modelu, regularyzacja, funkcje Hermita.