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Numerical simulation in processing of experimental data on mechanical spectroscopy of materials

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Expansion of complex mechanical spectroscopy spectra into components defined by dependences with Debye maxima and hysteresis curves has been proposed. An algorithm for approximation of experimental data basing on generalized Debye functions has been developed.

Предложено разложение сложных спектров механической спектроскопии на составляющие, которые определяются зависимостями с дебаевскими максимумами и гистерезисными кривыми. Разработан алгоритм приближения экспериментальных данных на основе обобщенных дебаевских функций.

The mechanical spectroscopy suggests examination of mechanical systems exhibiting both weak and strong nonlinearity to provide information on the properties and structure state thereof. Temperature, frequency, and amplitude spectra are used. The engineering materials show as a rule complex relaxation spectra presenting a superposition of several non-elastic processes at different mechanisms of the processes running. A necessity arises to analyze the mechanical spectra, to expand those into components as well as to describe the object physical model. It is just the description using mathematical characteristics with parameters adequate to the nature of processes occurring in the material that will be the most comprehensive.

Let a temperature dependence of Q^{-1} be presented by a background and a sum of m maxima [1]:

$$Q^{-1}(T) = Q_0^{-1}\exp(-H_\varphi/RT) + \sum_{k=1}^{m} Q_{m(k)}^{-1}/(\mathrm{ch})(H_k/R)(T^{-1} - T_{m(k)}^{-1}), \quad (1)$$

where the index k numbers individual maxima; Q_0^{-1} is the pre-exponential background factor; H_φ, the activation energy; $T_{m(k)}$, temperature of the maximum at the specified frequency f. The spectrum consists of a limited number of maxima having the regular Debye shape with the broadening parameter $\beta = 0$.

In most cases, the measured maxima of Q^{-1} are wider that the Debye peak due to superposition of several relaxation processes, each having its proper relaxation time τ_p. The maximum obtained in experiment can be expanded into a sum of Debye ones if the relaxation time spectrum is discrete, that is, the number of processes is small enough and the τ_p values corresponding thereto differ significantly. When the spectrum is continuous [2], the distribution parameter β is introduced that, as well as the τ_p parameter (relaxation time) and H (activation energy), is an important characteristic of physical processes. The β value defines changes in the Q^{-1} maximum height and shape as compared to the Debye one having $\beta = 0$. Even at low β values when the peak broadening $r_{2(\beta)}$ does not exceed 1.25, the H value (determined from the peak half-width [1]) becomes changed substantially. Then the items of (1) are changed by functions [1]

$$g_k = \frac{Q^{-1}}{Q^{-1}_{m(k)}} = \mathrm{ch}^{-1}\left(\frac{H_k}{r_2(\beta_k)R}\left(\frac{1}{T} - \frac{1}{T_{m(k)}}\right)\right). \quad (2)$$

The higher is grad T, the more broadens the maximum while its height is lowered. The decrease of $Q^{-1}_{m(k)}$ is the more, the higher is the activation energy H_k characterizing the maximum to be measured [3]. The H_k values determined using different methods can be different (sometimes by a factor of two) [4], because all the methods in use were elaborated under assumption that the maximum has the Debye shape [1]. It is impossible to assess the errors of H_k determination as well as to expand the spectrum into its components g_k when the shape variations of the items g_k are not known exactly. Therefore, of a great importance is the choice of a mathematical curve having a more general form than the function of (2) type and including parameters having a definitive physical sense at the same time. Let a function $\varphi_k(x) = \varphi_k(x, A_k, \alpha_k, \beta_k, \gamma_k, x_k)$ be chosen as such a function (with abstract parameters used in order to provide independence of the computer program of any specific problem):

$$\varphi_k(x) = \frac{A_k e^{-\alpha_k(x-x_k)}}{1 + \gamma e^{-\beta_k(x-x_k)}}, \quad (3)$$
$$A_k > 0, \alpha_k > 0, \beta_k > 0, \gamma_k > 0,$$

that coincides with the Debye curve for $\beta_k = 2\alpha_k$, $\gamma_k = 1$, $A_k = 2$:

$$\varphi_k(x,2,\alpha_k,2\alpha_k,1,x_k) = \frac{2e^{-\alpha_k(x-x_k)}}{1 + e^{-2\alpha_k(x-x_k)}} = \quad (4)$$
$$= \mathrm{ch}^{-1}(x,\alpha_k,x_k)$$

as well as coincides with the curve (2) (the Debye one at a broadened peak) if $\beta_k = 2\alpha_k$, $A_k \neq 2$ and $\gamma_k \neq 1$. When the absolute value of the curve $\varphi_k(x)$ change rates in the points positioned to left of its maximum and to right thereof are different, then $\beta_k \neq 2\alpha_k$. Such dependences are observed for amplitude-dependent internal friction when studying magneto-mechanical dampings in magnet fields of different strength [5, 6]. It is easy to prove that the function $\varphi_k(x)$ has a maximum only when $\beta_k > \alpha_k > 0$; the maximum point is determined by formulas

$$x_{\max} = x_k - \frac{1}{\beta_k}\ln\frac{\alpha_k}{\gamma_k(\beta_k - \alpha_k)}, \quad (5)$$
$$\varphi_{max,k} = A_k(1 - \alpha_k/\beta_k)[\gamma_k(\beta_k/\alpha_k - 1)]^{-\alpha_k/\beta_k}.$$

Note that $\varphi_k(x_k) = A_k(1 + \gamma_k)^{-1}$ and $x_{max} = x_k$ only when $\gamma_k = (\beta_k/\alpha_k - 1)^{-1}$. The curve symmetry with respect to $x = x_{max} = x_k$ is possible only at $\beta_k = 2\alpha_k$.

When studying the concentration dependences of the Snook hydrogen maximum in niobium [7] (non-elastic Gorsky relaxation [2]), an unsymmetrical experimental curve of (3) type has been obtained.

The relaxation maxima caused by interstitial atoms in hexagonal metals exhibit some singularities. The maximum shape is close to the Debye one both in polycrystals [8, 9] and in single crystals [10]. In high purity metals, no maxima are observed at all at low concentrations of interstitial atoms [11]. If the $\varphi_k(x)$ function is chosen as the mathematical model, then $\alpha_k \geq \beta_k > 0$ should be posed.

The amplitude dependence of internal friction associated with dislocation motion [12, 13] may be of linear, exponential, or more complex character [14–18]. As the modeling function, let $\varphi_k(x)$ for $\beta_k = \alpha_k$ be chosen having two horizontal asymptotes: $\varphi_{k,0}$ when $x \to +\infty$ and $\varphi_{k,1} = A_k/\gamma_k$ when $x \to -\infty$. A pair of such functions $\varphi^{(1)}_k = \varphi_k(x, A_k, \alpha_k, \beta_k, \gamma_k, x^{(1)}_k)$, $\varphi^{(2)}_k = \varphi_k(x, A_k, \alpha_k, \beta_k, \gamma_k, x^{(2)}_k)$ with biased centers $x^{(1)}_k \neq x^{(2)}_k$ forms a hysteresis loop. When studying continuous spectra, arbitrarily broadened maxima can be constructed using the difference of those functions:

$$\psi_k(x) = \frac{A_k e^{-\alpha_k(x-x^{(1)}_k)}}{1 + \gamma_k e^{-\alpha_k(x-x^{(1)}_k)}} - \frac{A_k e^{-\alpha_k(x-x^{(2)}_k)}}{1 + \gamma_k e^{-\alpha_k(x-x^{(2)}_k)}}. \quad (6)$$

The function $\psi_k(x)$ attains its maximum in the point

$$x_{\max} = \frac{x^{(1)}_k + x^{(2)}_n}{2} + \frac{1}{\alpha_k}\ln\gamma_k;$$

$$\psi_{max,k} = \frac{A_k}{2\gamma_k} \frac{\mathrm{sh}(\alpha_k \frac{x^{(1)}_k - x^{(2)}_k}{2})}{\mathrm{ch}^2(\alpha_k \frac{x^{(1)}_k - x^{(2)}_k}{4})}.$$

When $\gamma_k = 1$, then $x_{\max} = \frac{x_k^{(1)} + x_k^{(2)}}{2}$. The function $\psi_k(x)$ has a Debye character but with more independent parameters, thus making it possible to describe the physical process in a more comprehensive fashion (the Debye curve has three independent parameters, the $\psi_k(x)$, four ones). A generalization of the $\psi_k(x)$ dependence is the function

$$\xi_k(x) = \frac{\alpha_{1k} e^{-\alpha_k x}}{1 + \gamma_{1k}\alpha_{1k} e^{-\alpha_k x}} - \frac{\alpha_{2k} e^{-\beta_k x}}{1 + \gamma_{2k}\alpha_{2k} e^{-\beta_k x}},$$

$$\frac{\alpha_{1k}}{\gamma_{1k}} = \frac{\alpha_{2k}}{\gamma_{2k}},$$

allowing to study characteristics of more complex forms as compared to the Debye one (asymmetric curves with respect to $x = x_{max}$).

Substituting functions $\varphi_k(x)$, $\psi_k(x)$, $\xi_k(x)$ for Debye ones $q_k(x,b_k,x_k) = \frac{1}{a_k + b_k(x - x_k)^2}$ in (1) and approximating Q^{-1} according to various criteria, we obtain the spectrum expansion into components making it possible to consider the physical processes if the parameters have a physical sense.

It is just the least square method that is chosen usually as the approximation criterion (for experimental curves set discretely or continuously). Such a choice is justified, since, first, it makes it possible to process experimental data including errors and, second, the method algorithm is easy to be programmed. The methods drawbacks are a strong dependency on the selection of initial parameters and a slow convergence. More robust results can be obtained using a criterion with weight coefficients, if there is a confidence that the specified section of the temperature or frequency dependences image the actual process at a highest accuracy. Note that if the items of (1) are linearly independent functions in the section under study, then the approximation will be always highly accurate although it may be physically senseless. Therefore, a mathematical model (that is, the choice of mathematical functions) will be adequate to the actual process only when the parameters are proven in experiment.

We have developed an algorithm to approximate the experimental curves by a polynomial

$$P_n(x) = A_n + \sum_{k=1}^{n} A_k q_k(x,b_k,x_k)$$

with basic Debye functions (parameters A_0, $\{A_k, b_k, x_k\}$ are abstract quantities, $b_k > 0$, $k = 1, 2,...n$). Let an experimental curve be specified by a data set (X_i,Y_i), $i = 0,1...m$, $m >> n$. It is necessary to determine the minimum number of items n and parameters A_0, $\{A_k, b_k, x_k\}$, $k = 1,...n$ under condition

$$\delta_n = \min\sum_{i=0}^{m}(P_n(x_i) - Y_i)^2 < \varepsilon_n, \quad \mathbf{c}_n \in \Omega, \tag{7}$$

where ε_n is the pre-specified error, $\mathbf{c}_n = \{A_0,\{A_k,b_k,x_k\}, \quad k = 1...n\}$; $\Omega = \{A_0, \quad A_1,..., A_n \in R; \quad b_k \geq b_0 > 0, \quad x_k \geq 0, \quad k = 1...n\}$, the convex closed set. The problem (7) is a nonlinear one, so that it is necessary to prespecify the initial parameters a priori or basing on the experimental curve shape.

The determination procedure for the parameters consists in the determination of the initial vector (**A**,**b**,**w**) from the characteristics of the maximum peak (x_k is the peak center, b_k defines its half-width) and optimization of the deviation δ_n until the condition (7) will be met. At each procedure step, the least square method was used in the vicinity of the maximum peak for successive rough determination of each b_k parameter. When the parameters (A_k, b_k, x_k) were determined, an algorithmically new network function $\{X_k, \ Y_k(x)\}$ was constructed by subtracting the Debye function $q_k(x)$. Using the Newton method, the nonlinear system of equations was solved making it possible to find approximately $\min\delta_n(\mathbf{c}_n)$. This was the end of the first procedure step of a $P_n(x)$ polynomial construction. At the second step, the components (b_k, x_k) of the vector $\mathbf{c}_n$ were fixed and the function $\delta_n(\mathbf{a}_n)$, $\mathbf{a}_n = (A_0, A_1, ...A_n)$ was minimized as the convex function of the parameter vector $\mathbf{a}_n$, thus allowing to find the vector $\mathbf{a}_n$ when the components (b_k, x_k), $k = 1,...,n$ were specified. The procedure was repeated until the iteration convergence.

The construction algorithm for a polynomial with Debye functions $q_k(x)$ can be used to construct the polynomial $P_n(x)$ with basis functions $\varphi_k(x)$, $\psi_k(x)$, $\xi_k(x)$. The algorithm was generalized for the multidimensional case using tensor concepts. Figs. 1, 2 show the steps of experimental data processing, that is, the spectrum expansion into Debye components. Note that the linearization of nonlinear equations in the least square method [1] can be used only to obtain the initial ap-

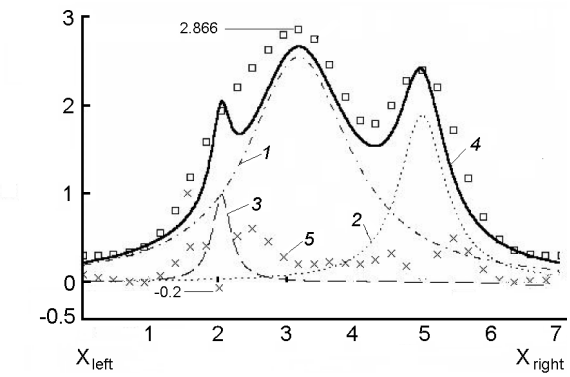

Fig. 1. Expansion of a spectrum into components: square — experimental, *1*—peak 1(x), *2* — peak 3(x), *3* — peak 4(x), *4* — approach (x); *5* — best.

proximations. This is due to a linear convergence rate is observed at the linearization.

Thus, functions have been proposed that generalize the Debye characteristics. Those functions have been used to expand the mechanical spectra into components and to analyze the physical model of an object. The multidimensional functions can be used to construct the numerical-analytical methods for solution of boundary problems being mathematical models of magnet-mechanical processes in materials [19].

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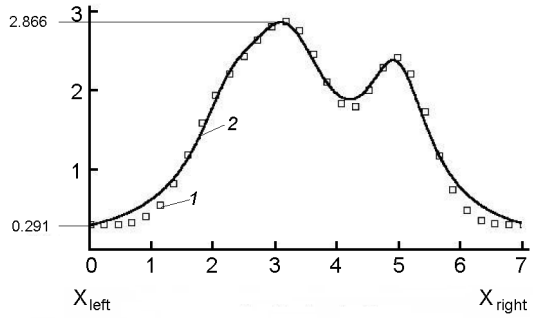

Fig. 2. Resultant characteristic: square – experimental, solid line – approach (x)

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Чисельне моделювання при обробці експериментальних даних механічної спектроскопії матеріалів

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Запропоновано розкладання складних спектрів механічної спектроскопії на складові, що визначаються залежностями з дебаївськими максимумами та гістерезисними кривими. Розроблений алгоритм наближення експериментальних даних на основі узагальнених дебаївських функцій.