approximate solution $P^{\alpha}(U)$ to equation (5) that satisfies the natural requirements that are embedded in the meaning of an approximate solution by the physical determinism of the phenomenon described by this equation and the possibility of physical interpretation of the solution, namely the conditions

$$P^{\alpha}(U) \to \hat{P}(U) \text{ at } \upsilon \to 0, \tag{9}$$

it is necessary from the entire set of formal solutions $P(U)$ that satisfy condition (7) to select a function $P^{\alpha}(U)$ that satisfies condition (9). This can be done if there is additional information, at least of a qualitative nature, regarding the desired solution. We will assume that the desired spectrum $P^{\alpha}(U)$ does not have a fine structure, i.e. we can assume that the solution to the problem under consideration is a smooth function. As a measure of smoothness, consider the quantity

$$\Omega[P] = \int\limits_{U_{\min}}^{U_{\max}} \left\{ \xi(U) \cdot P^2(U) + \chi(U) \cdot \left(\frac{dP(U)}{dU} \right)^2 \right\} dU , \tag{10}$$

where $\xi(U)$ and $\chi(U)$ are given non-negative continuous functions satisfying the condition $\xi^2(U) + \chi^2(U) \ne 0$ for any $U \in (U_{\min}, U_{\max})$. This definition of smoothness is consistent with the visual representation of the smoothness of the graphs of functions.

Following [7], as the required spectrum $P^{\alpha}(U)$, we will choose from the family of approximate solutions $P(U)$ a function with the greatest smoothness (minimum fine structure). Mathematically, this problem is reduced to finding such a function $P^{\alpha}(U)$ that will achieve the minimum of the functional (10). The solution of such a problem for a conditional extremum is reduced to a problem for an unconditional extremum of a functional

$$M_{\alpha}[P,Z] = \int\limits_{T_{\min}}^{T_{\max}} \left\{ \int\limits_{U_{\min}}^{U_{\max}} K(T,U) P(U) dU - Z(T) \right\}^2 dT + \alpha \Omega[P], \tag{11}$$

where $\alpha > 0$ is the regularization parameter, which can be determined by a given accuracy υ and, therefore, depends on υ, i.e. $\alpha = \alpha(\upsilon)$. It can be shown [7] that $\alpha(\upsilon)$ is the function that convex downward, besides there is an estimate

$$\alpha \le \frac{\upsilon \|A\|^2}{\|z\| - \upsilon} . \tag{12}$$

The solution to the minimum problem for functional (11) is called a regularized (approximate) solution $P^{\alpha}(U)$ to equation (5) and can be found from the Euler equation for the functional M_{α}:

$$\alpha \left\{ \xi(U) \cdot P(U) - \frac{d}{dU} \left[\chi(U) \cdot \frac{dP(U)}{dU} \right] \right\} + \int\limits_{U_{\min}}^{U_{\max}} \bar{K}(U,t) P(t) dt = g(U), \tag{13}$$

with boundary conditions

$$\frac{dP}{dU}(U_{\min}) = 0, \qquad \frac{dP}{dU}(U_{\max}) = 0 , \tag{14}$$

where $\bar{K}(U,t) = \int\limits_{T_{\min}}^{T_{\max}} K(T,U) \cdot K(T,t) dT$, a $g(U) = \int\limits_{T_{\min}}^{T_{\max}} K(T,U) \cdot Z(T) dT$.

Another difficulty lies in the fact that the right-hand side of (5) in our problem is the result of an experiment, i.e. known on the grid by $T: \{T_1, \cdots, T_N\}$. With this right-hand side, equation (5) has no solution at all, understood in the classical sense, i.e. determined by the formula $p = A^{-1}z$ (A^{-1} is the operator inverse to the operator A) in equation (5) since the kernel $K^{d,m}(T,U)$ has a continuous derivative with respect to T and, therefore, the right-hand side must also have a continuous derivative with respect to T. This means that in this formulation of the problem, the exact solution $\hat{P}(U)$ of this equation with an approximately known right-hand side $Z^{d,m}(T) \ne \hat{Z}^{d,m}(T)$ cannot be taken as an

approximate to $P(U)$ solution of equation (5), since such a solution may not exist. In this regard, it becomes necessary to pass from the continuous initial problem of finding regularized approximate solutions (5) to its discrete analogue. This transition is carried out by discretizing the boundary value problem for the Euler equation by solving the resulting SLAE [7]. Following the variational approach, we take a discrete analogue of stabilizer (10) and form an analogue of the smoothing functional (11). Then we turn to his Euler equation (13), which will represent the regularized SLAE. The solution to this system (with an appropriately selected regularization parameter) will be an approximate solution to the original problem.

For simplicity of further consideration, we will accept $\xi(U) \equiv \xi$ and $\chi(U) \equiv \chi$ (ξ and χ are positive numbers). Then the difference analogue of Eq. (13) on a uniform grid of N nodes by U in increments of $\Delta U = \dfrac{U_{\max} - U_{\min}}{N-1}$ will have the following form:

$$\sum_{j=2}^{N-1} \overline{K}_{ij} \cdot P_j \cdot \Delta U + \frac{\overline{K}_{i1} \cdot P_1 + \overline{K}_{iN} \cdot P_N}{2} \Delta U + \alpha \xi \cdot P_i + a\chi \frac{2P_i - P_{i-1} - P_{i+1}}{(\Delta U)^2} = g_i, \ i = 1, \cdots, N, \tag{15}$$

where $U_i = U_{\min} + (i-1) \cdot \Delta U$, $P_i = P(U_i)$, $g_i = g(U_i)$, $\overline{K}_{ij} = \overline{K}(U_i, T_j)$. In this expression the integral is replaced by the corresponding integral sum by the trapezoidal formula, and $\dfrac{d^2 P(U)}{dU^2}$ by the corresponding difference relation.

For simplicity, we will assume that the number of grid nodes by T is also N, and the step $\Delta T = \dfrac{T_{\max} - T_{\min}}{N-1}$. Then $T_j = T_{\min} + (j-1) \cdot \Delta T$ and the values $\overline{K}_{ij}$ and g_i can also be calculated using the trapezoidal formula:

$$\overline{K}_{ij} = \sum_{m=2}^{N-1} K_{mi} \cdot K_{mj} \cdot \Delta T + \frac{K_{1i} \cdot K_{1j} + K_{Ni} \cdot K_{Nj}}{2} \Delta T \ \text{and} \ g_i = \sum_{j=2}^{N-1} K_{ji} \cdot Z_j \cdot \Delta T + \frac{K_{1i} \cdot Z_1 + K_{Ni} \cdot Z_N}{2},$$

where $Z_j = Z(T_j)$ and $K_{ji} = K(T_j, U_i)$.

For $i = 1$ and $i = N$, (15) contains unknown values of P_0 and P_{N+1}. To satisfy the boundary conditions (14), we put $P_0 = P_1$ and $P_{N+1} = P_N$.

System (15) can be written in matrix form with respect to the vector $P = (P_1, \cdots P_N)$:

$$B \cdot P + \alpha C \cdot P = g, \tag{16}$$

where the vector $g = (g_1, \cdots, g_N)$, the matrix B has the form:

$$B = \begin{bmatrix} \dfrac{\overline{K}_{11}}{2}\Delta U & \overline{K}_{12}\Delta U & \cdots & \overline{K}_{1N-1}\Delta U & \dfrac{\overline{K}_{1N}}{2}\Delta U \\ \vdots & \vdots & & \vdots & \vdots \\ \dfrac{\overline{K}_{N1}}{2}\Delta U & \overline{K}_{N2}\Delta U & \cdots & \overline{K}_{NN-1}\Delta U & \dfrac{\overline{K}_{NN}}{2}\Delta U \end{bmatrix},$$

and αC is a symmetric matrix of the form:

$$\begin{bmatrix} \alpha\left(\xi + \dfrac{\chi}{(\Delta U)^2}\right) & -\dfrac{\alpha\chi}{(\Delta U)^2} & 0 & 0 & \cdots & 0 \\ -\dfrac{\alpha\chi}{(\Delta U)^2} & \alpha\left(\xi + \dfrac{2\chi}{(\Delta U)^2}\right) & -\dfrac{\alpha\chi}{(\Delta U)^2} & 0 & \cdots & 0 \\ 0 & -\dfrac{\alpha\chi}{(\Delta U)^2} & \alpha\left(\xi + \dfrac{2\chi}{(\Delta U)^2}\right) & -\dfrac{\alpha\chi}{(\Delta U)^2} & \cdots & 0 \\ & \bullet & \bullet & \bullet & & \\ 0 & \cdots & 0 & 0 & -\dfrac{\alpha\chi}{(\Delta U)^2} & \alpha\left(\xi + \dfrac{\chi}{(\Delta U)^2}\right) \end{bmatrix}$$

In our case, boundary conditions (14) can be supplemented by conditions of the form: $P(U_{\min}) = P(U_{\max}) = 0$, in this case, the matrix αC will have the form:

$$\begin{bmatrix} 0 & -\dfrac{\alpha\chi}{(\Delta U)^2} & 0 & 0 & \cdots & 0 \\[2ex] 0 & \alpha\left(\xi + \dfrac{2\chi}{(\Delta U)^2}\right) & -\dfrac{\alpha\chi}{(\Delta U)^2} & 0 & \cdots & 0 \\[2ex] 0 & -\dfrac{\alpha\chi}{(\Delta U)^2} & \alpha\left(\xi + \dfrac{2\chi}{(\Delta U)^2}\right) & -\dfrac{\alpha\chi}{(\Delta U)^2} & \cdots & 0 \\[1ex] & \bullet & \bullet & \bullet & & \\[1ex] 0 & \cdots & 0 & 0 & -\dfrac{\alpha\chi}{(\Delta U)^2} & 0 \end{bmatrix}.$$

Thus, the problem is reduced to solving the SLAE with respect to the vector $P = (P_1, \cdots P_N)$.

DISCUSSION OF THE RESULTS

The spectral function $P^T(U)$ found by the Tikhonov regularization method has a maximum in the region of 0.04 eV corresponding to the α-peak of acoustic absorption and largely coincides with the quasi-Gaussian function $P^G(U)$ empirically selected in [3] (Fig. 2).

In this case, the position of the maximum of the $P^T(U)$ depends on the structural state of the sample. This fact numerically and qualitatively correlates with the conclusions of [3] about the change in the effective value of the activation energy $U_{eff} = \int\limits_0^\infty UP(U)dU \cong U_0 + \dfrac{D^2}{U_0}$ due to the change in the statistical scatter characterized by the dispersion parameter D (Table).
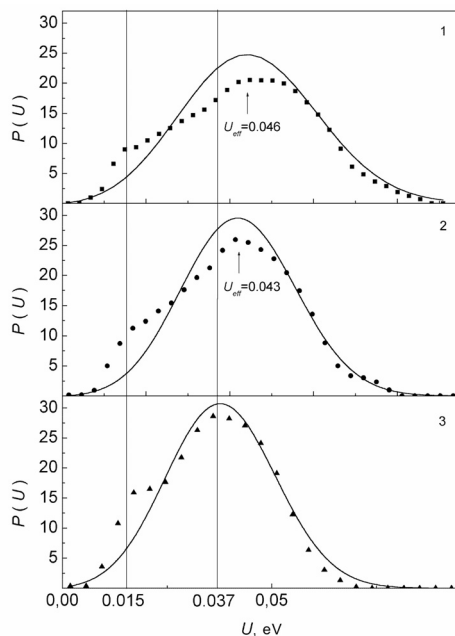
Figure 2. Spectral functions (distribution functions of activation energy values) $P^G(U)$ and $P^T(U)$ for various structural states of the sample (the numbering of structural states corresponds to that shown in Fig. 1):

■, ●, ▲ – the spectral function $P^T(U)$ which was found by the Tikhonov regularization method; **solid lines** - spectral function $P^G(U)$ calculated by formula (4) for the quasi-Gaussian distribution function with an appropriate choice of values U_0 and D

The spectral function $P^T(U)$ also has a feature in the form of a second mode in the region of 0.015 eV; the position of this feature is practically independent of the structural state of the sample. If we assume that this feature corresponds to a relaxation resonance (α'-peak) with the same value of τ_0 as the main resonance, then it should correspond to a feature in the form of a peak on temperature dependence of the δ and a step on temperature dependence of the $\Delta M/M_0$ in the region of 14-16 K (at an oscillation frequency sample 88 kHz). In [3] these features were not found experimentally, which may be associated with a significant broadening of the main relaxation resonance at a temperature of ≈ 54 K. However, in one form or another, the α'-peak was repeatedly observed by various

authors [8]-[19]. For example, in [10] a resonance in the region of 17 K was found in Fe single crystal with an orientation <100>. It was shown in [16] that annealing leads to a narrowing and a shift toward lower temperatures of the α-peak and the appearance of a α'-peak that was not observed in the initial curves. It was shown in [17], [18] that the α'-peak should be characterized by the same period of attempts as the α-peak and have a value of the order of 10^{-11} s.

Table. Acoustic relaxation parameters in a single-crystal sample of high-purity iron with orientation <731> in various structural states, according to the data of [3], [4]:

Relaxation parameters	Structural state of the sample		
	1	**2**	**3**
U_0^{α} , eV	0.037		
D^{α} , eV	0.0177	0.0143	0.0136
$C_r \Delta_0$	0.00472	0.00271	0.00180
U_{eff}^{α} , eV	0.046	0.043	0.042
$\tau_0^{\alpha} \cdot 10^{11}$, s	2.4		
$U_0^{\alpha'}$, eV	0.015		

In order to detect the α'-peak in Fe single crystals of the <731> orientation, additional experimental studies were carried out in [4]. A sample in the form of a thin plate was made from the same single crystal as in [3]. The acoustic properties of this sample were studied in the temperature range 4.5-150 K. It was found that in the undeformed sample α and α' peaks are not observed, deformation leads to the appearance of α-peak localized at 35 K and its α' satellite at a temperature of 13 K. Subsequent annealing at 320 K leads to a decrease in the height of the α peak, narrowing and shifting to lower temperatures, while the α'-peak becomes more pronounced. The analysis performed in [4] made it possible to establish the microscopic nature of the α' -peak and determine the corresponding activation energy of an elementary relaxator $U_0^{\alpha'} = 0.015$ eV; it was also shown that the activation energy values corresponding to the α'-peak have a small statistical spread, which practically does not change with a change in the structural state sample.

Thus, the values of the activation energy $U_0^{\alpha} = 0.037$ eV and $U_0^{\alpha'} = 0.015$ eV determined experimentally in [4] corresponding to the α-peak and its α' satellite are in good agreement (taking into account the statistical spread) with the positions of the peaks on the dependence $P^T(U)$ obtained by solving the inverse problem, and its substitution into expression (3) makes it possible to exhaustively describe the experimentally observed spectrum of low-temperature acoustic relaxation in iron (Fig. 1).

CONCLUSIONS

A mathematical procedure for processing experimental data is proposed that allows solving the inverse problem of low-temperature mechanical spectroscopy - to restore the energy spectrum of relaxation by analyzing the temperature dependence of acoustic absorption.

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СПЕКТР ЕНЕРГІЇ АКТИВАЦІЇ НИЗЬКОТЕМПЕРАТУРНОЇ АКУСТИЧНОЇ РЕЛАКСАЦІЇ В МОНОКРИСТАЛІЧНОМУ ЧИСТОМУ ЗАЛІЗІ. ВИРІШЕННЯ ЗВОРОТНОЇ ЗАДАЧІ МЕХАНІЧНОЇ СПЕКТРОСКОПІЇ МЕТОДОМ РЕГУЛЯРИЗАЦІЇ ТИХОНОВА

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При вивченні температурних залежностей акустичного поглинання та модуля пружності часто спостерігаються релаксаційні резонанси - піки поглинання, яким на температурній залежності модуля пружності відповідає характерна сходинка. Вважається, що виникнення таких релаксаційних резонансів пов'язано з наявністю в структурі матеріалу елементарних мікроскопічних релаксаторів, що взаємодіють з досліджуваною коливальною модою механічних коливань зразка. В достатньо досконалому матеріалі такий процес характеризується часом релаксації τ, а у реальному матеріалі з дефектами - спектром часу релаксації $P(\tau)$. Найчастіше такі релаксаційні процеси мають термічно активований характер і час релаксації $\tau(T)$ визначається співвідношенням Ареніуса $\tau(T) = \tau_0 \exp(U_0/kT)$, а характеристиками процесу будуть U_0 - енергія активації, τ_0 - період спроб, Δ_0 - характерний елементарний внесок окремого релаксатора у динамічний відгук матеріалу та їх спектри. В області низьких температур $kT \ll U_0$ статистичним розподілом параметрів τ_0 та Δ_0 з експоненційною точністю можна знехтувати, а релаксаційний внесок у температурні залежності поглинання та динамічного модуля пружності матеріалу будуть визначатися тільки спектром енергій активації $P(U)$ мікроскопічних релаксаторів. Основна задача механічної спектроскопії при аналізі таких релаксаційних резонансів зводиться до визначення U_0, τ_0, Δ_0 та $P(U)$. У роботі показано, що проблема знаходження спектральної функції $P(U)$ для енергії активації акустичної релаксації в реальних кристалах з дефектами, зводиться до вирішення інтегрального рівняння Фредгольма I роду з приблизно відомою правою частиною і відноситься до класу некоректно поставлених задач. Запропоновано метод визначення $P(U)$ виходячи з експериментальних температурних залежностей акустичного поглинання чи модуля пружності, що ґрунтується на алгоритмі тихоновської регуляризації. Встановлено, що акустична релаксація у чистому монокристалічному залізі в області температур 5÷100 К характеризується двомодовою спектральною функцією $P(U)$ з максимумами в області 0.037 еВ та 0.015 еВ, що відповідають α-піку та його α' сателіту.

КЛЮЧОВІ СЛОВА: акустична релаксація, регуляризація Тихонова, спектр енергії активації, акустичне поглинання, модуль пружності