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DESCRIPTION OF THE IRREVERSIBLE DEFORMATION OF SHAPE-MEMORY MATERIALS IN TERMS OF THE TWO-LEVEL PHENOMENOLOGICAL MODEL

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The two-level phenomenological model of the nonlinear deformation of polycrystals is extended to describe and predict the irreversible deformation of advanced shape-memory materials. The effect of various groups of residual microstresses on the deformation process is taken into account. The model is used to describe and predict deformations of shape-memory materials in cyclic thermomechanical tests, and its effectiveness is demonstrated.

Key words: *martensitic transformation, shape-memory effect, nonlinear deformation, phenomenological model.*

Under complex operation conditions, contemporary polycrystalline materials usually exhibit special properties related to irreversible deformation of defect nature: anomalous behavior of the plastic limit, strain-rate effects, anomalous creep, etc. Moreover, deformation processes of martensitic nature — reversible martensitic transformations (MTs) — are observed, and multiaspect interaction of various deformation processes occurs. For these reasons, the classical theories of the nonlinear deformation of polycrystals fail in many cases. It is therefore of prime importance to develop generalized theories that would provide an adequate mathematical description of deformation processes in advanced materials.

Among the various approaches to solving the above-mentioned problem, the slip concept [1] based on the physically substantiated assumption of the shear nature of microlevel deformation is worth noting. Owing to the universal nature of this assumption, the model can be applied to various deformation processes. Among the theories that elaborate and extend this concept is the two-level theory of plasticity [2], which combines the essentials of slip theory and the concept of flow with a singular loading surface. The constitutive relations of this model are simpler than those in slip theory and can be extended to deformation phenomena. The main components of the deformation process in advanced shape-memory materials were generally studied in [3–7]. Among these components are reversible deformation of martensitic nature, irreversible plastic deformation of defect origin, elastic deformation, and thermal deformation. The present paper deals with the most complex component of the deformation process for shape-memory materials — irreversible deformation of defect origin. The interaction of deformation processes of different natures, including the action of residual microstresses, is taken into account.

In the model proposed, it is assumed that the strain magnitude depends on the displacement of planes in Ilyushin's five-dimensional deviatoric space and each plane corresponds to a certain slip system. Following the concept of [1], we assume that the slip system is a unique system for each distinguished volume that corresponds to the lower level of the model. Moreover, we assume that separate crystalline elements do not interact, and the polycrystalline nature of the medium is displayed by different orientations of the distinguished volumes and, hence, slip systems and corresponding planes in the deviatoric space.

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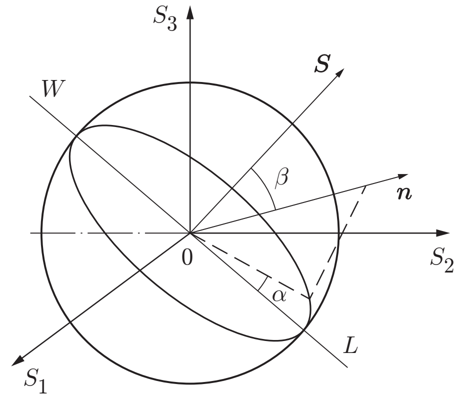

Fig. 1

The lower-level scale depends on the physical nature of the phenomena studied. In theories of this class, this dimension is not fixed [8]; the distinguished volume is treated as a representative elementary volume over which averaging is performed. The representative nature of the distinguished volume implies that its characteristics are themselves the results of averaging over separate smaller-scale elements: therefore, this volume can be referred to as a "mesovolume."

The planes of the deviatoric space move translationally, and the translation magnitude characterizes an elementary deformation act. In the combined space of stresses and strains, the components of the macrostress and macrostrain vectors are related to the components of the corresponding deviators by the well-known relations [9]:

$$\varepsilon_1 = (\sqrt{3}/2)e_{xx}, \quad \varepsilon_2 = (\sqrt{2}/2)(e_{yy} - e_{zz}), \quad \varepsilon_3 = \sqrt{2}\,e_{xy}, \quad \varepsilon_4 = \sqrt{2}\,e_{yz}, \quad \varepsilon_5 = \sqrt{2}\,e_{xz},$$

$$S_1 = (\sqrt{3}/2)S_{xx}, \quad S_2 = (\sqrt{2}/2)(S_{yy} - S_{zz}), \quad S_3 = \sqrt{2}\,S_{xy}, \quad S_4 = \sqrt{2}\,S_{yz}, \quad S_5 = \sqrt{2}\,S_{xz}.$$

If loading occurs in the three-dimensional subspace of the above-mentioned deviatoric space determined by the components of the vector S_1, S_2, and S_3, the strain is uniquely determined from the translation of the traces of the planes in the three-dimensional space; the relationship between a plane of the five-dimensional space (with normal $\boldsymbol{M}$) and its trace in the three-dimensional subspace (with normal $\boldsymbol{n}$) is given by the relation $M_k = n_k \cos\lambda$ ($k = 1$, 2, 3), where λ is the angle between the normals $\boldsymbol{M}$ and $\boldsymbol{n}$.

The direction cosines of the normal to the plane of three-dimensional subspace are specified in a special spherical coordinate system related to the loading vector $\boldsymbol{S}$ via the angles α and β: the angle β is the angle between $\boldsymbol{S}$ and $\boldsymbol{n}$, and α is the angle between the projection of $\boldsymbol{n}$ onto the plane W normal to $\boldsymbol{S}$ and intersecting the coordinate origin and the line L of intersection of W with the coordinate plane S_1OS_2 (Fig. 1). The coordinate system proposed and its related averaging method allow one to bring the loading vector into coincidence with the coordinate axis and represent the strain-vector components in finite form for an arbitrary proportional load [2–5].

To describe irreversible strain of defect nature at the lower structural level of the model in a variable temperature-force field, one can use the formula [10, 11]

$$d\Psi = d\varphi - K_0(T, S)\Psi\, dt, \tag{1}$$

where φ is the irreversible-strain intensity, Ψ is the hardening intensity or defect intensity, which is an averaged continuous characteristic of crystal lattice defects during deformation. The irreversible-strain intensity is an averaged continuous characteristic of the crystal lattice distortion during deformation. In the model in question, it is determined by the load-induced displacement of the planes relative to the initial location and specified in the mesovolume with the normal $\boldsymbol{M}$. The parameter K_0 depends on the temperature level and magnitude of the loading vector, characterizes the rate of time-dependent microstructural processes (primarily, creep), and can characterize the vacancy concentration for specified loads and temperature [11]. Equation (1) implies that irreversible deformation stimulates the development of structural imperfections of polycrystals, and this process accompanies defect relaxation. This assumption, in particular, corresponds to the Beil–Orowan hypothesis [12]. Relation (1) can be used to describe "instantaneous" plastic strain and creep.

Irreversible deformation of dislocation nature leads to hardening of the material, which is determined by a change in the distance of the corresponding plane (with the normal $\boldsymbol{M}$) to the coordinate origin and depends on the initial deformability of the material (initial strength) and hardening; the latter is determined by the rate of variation of the applied load. Therefore, we have the relation

$$H_M = F(R, \Psi, R_M, I_M), \tag{2}$$

where H_M is the resultant distance to the plane with the normal $\boldsymbol{M}$. For irreversible deformation, the equality $H_M = (\boldsymbol{S}, \boldsymbol{M})$ holds. The argument R is the initial (at the onset of irreversible deformation) distance from the coordinate origin to the loading surface (LS). In accordance with [2], we have $R = \sqrt{2/3}\,\sigma_p$, where $\sigma_p(T)$ is the stress that causes irreversible distortions (in extension) dependent on temperature [7]. In this paper, we distinguish between two notions — the plastic limit and the irreversible-distortion limit. By the plastic limit is meant the stress at the beginning of distortion under sufficiently intense loading with allowance for rate effects and preceding cyclic tests.

The next two arguments in formula (2) determine the displacements of the plane with the normal $\boldsymbol{M}$ that correspond to strain hardening. The second argument (Ψ) accounts for hardening that depends on the applied temperature and can be eliminated under alternating loading, and the third argument (R_M), which does not decrease, characterizes the damage to the material [13]. The fourth argument (I_M) specifies additional displacements that can decrease (relax) with time and correspond to high-rate hardening. In formula (2), the third and fourth arguments — the relaxing and nonrelaxing parameters — account for the action of residual, so-called orientation microstresses in the plane with the normal $\boldsymbol{M}$. At the lower structural level of the model, these stresses can be produced by various physical factors related to the structural heterogeneity of the material [8]. In particular in shape-memory materials, they result from incomplete alignment of the crystal lattices of adjacent phases in mechanical martensitic transformations [14]. Accounting for the stresses capable of relaxation allows one to describe rate effects (in particular, transient creep). The quantities mentioned above can be found from the relations

$$dI_M = r_1\, d[(\boldsymbol{S}, \boldsymbol{M})] - h(T) I_M\, dt, \qquad I_m \equiv |I_M|,$$

$$dR_M = \begin{cases} r_2\, d[(\boldsymbol{S}, \boldsymbol{M})], & |dR_M| \geqslant 0, \\ 0, & |dR_M| < 0, \end{cases} \tag{3}$$

where $r_1, r_2 = \text{const}$.

From the aforesaid, the defect intensity is written as

$$\Psi = a[(H_M/\sqrt{2/3}\,\sigma_p(T))^2 - 1 - c_1 I_M - c_2 R_M], \tag{4}$$

where $a, c_1, c_2 = \text{const}$.

Irreversible deformation begins with displacements of the planes tangent to the loading surface. Initially, the loading surface is a sphere of radius $\sqrt{2/3}\,\sigma_p$. For further loading, the LS becomes a cone superimposed on a sphere of radius $\sqrt{2/3}\,\sigma_p$:

$$H_M = \begin{cases} \sqrt{2/3}\,\sigma_p(T), & \beta_1 \leqslant \beta \leqslant \pi/2, \\ S \cos\beta \cos\lambda, & 0 \leqslant \beta \leqslant \beta_1. \end{cases}$$

The vertex of the cone coincides with the end of the vector $\boldsymbol{S}$ and its base (the line of intersection of the cone and the sphere) is determined by the coordinate angle β_1; $0 \leqslant \beta_1 \leqslant \pi/2$; $\cos\beta_1 = \sqrt{2/3}\,\sigma_p/S$; $0 \leqslant \lambda \leqslant \lambda_1$; $\cos\lambda_1 = \cos\beta_1/\cos\beta$. During loading, the opposite (rear) side of the LS is also transformed according to the assumption

$$\Psi_{-M} = -g\Psi_M; \qquad I_{-M} = -gI_M; \qquad R_{-M} = -gR_M; \qquad g \leqslant 1.$$

The parameter σ_p can be written as

$$\sigma_p = \begin{cases} \sigma_{p1} = z_1 S_p, & M_s \leqslant T \leqslant M_s^\sigma, \\ \sigma_{p2} = z_1 K^{-1} \dfrac{M_s^\sigma - M_s}{T_{ml} - M_s^\sigma}\,(T_{ml} - T), & M_s^\sigma \leqslant T \leqslant T_{\text{con}}, \\ \sigma_{p3} = \sigma_{p2}(T_{\text{con}}), & T_{\text{con}} \leqslant T. \end{cases} \tag{5}$$

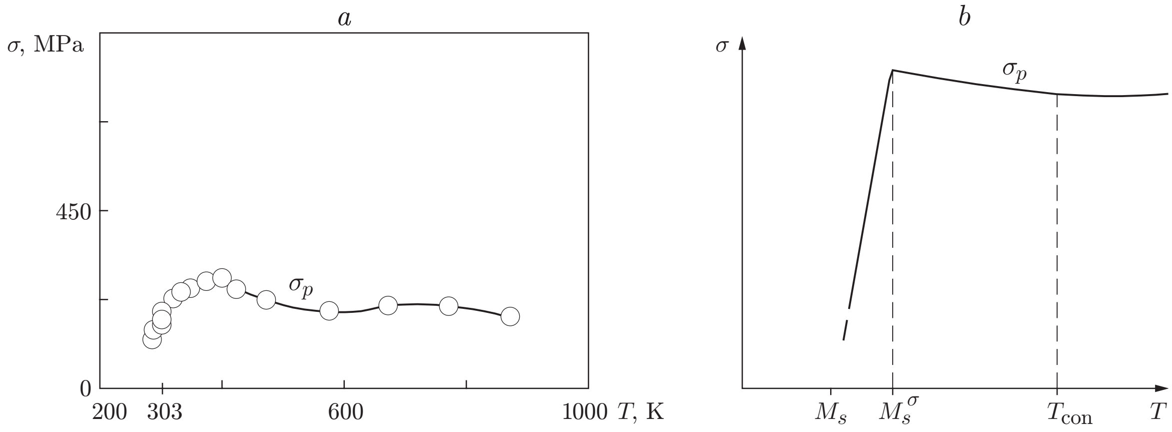

Fig. 2

In formula (5), $z_1 = \text{const}$, M_s is the characteristic temperature at the onset of the direct MT [8], M_s^σ is the maximum temperature at an anomalous dependence of the distortion limit on the temperature occurs (a linear increase in σ_p^i with temperature), $M_s^\sigma \geqslant M_s$, T_{con} and T_{ml} are the temperature parameters of the material ($T_{\text{con}} \leqslant T_{ml}$ and T_{ml} does not exceed the melting point of the material), S_p is the characteristic stress at the beginning of the direct mechanical martensitic transformation for single loading [4–5]; $S_p = (T - M_s)/K$. Figure 2a shows an experimental curve of σ versus T (experimental data of [14]), and Fig. 2b shows the qualitative dependence of σ on T that corresponds to formula (5).

At the macrolevel, the components of the irreversible strain vector of defect nature are given by

$$\varepsilon_k^p = \iiint\limits_{\Omega_1} d\Omega_1 \int\limits_t M_k\Big(\frac{d\varphi}{ds}\Big)\, ds; \qquad \Omega_1 = \Omega_1(\alpha, \beta, \lambda).$$

The irreversible-strain vector of the boundary of the region where deformation occurs is found form the condition $\Psi = 0$.

For high-rate loading regimes, it can be assumed that Eq. (4) is valid only if the irreversible-strain intensity increases, whereas relation (1) holds during the entire process of variation in the defect intensity (including the case of no increment in the irreversible strain). In the general case (for an arbitrary loading rate), we assume that Eq. (1) is valid during the entire testing process. That is, in all cases, the variation in the defect intensity (including relaxation) is described by relation (1).

Thus, in the model proposed, the deformation process is described by displacement of the corresponding set of planes of Il'yushin's five-dimensional deviatoric space.

In this formulation, as before [3–7], the constitutive relations of the model can be reduced to a form similar to the deformation theory of plasticity. A universal dependence between the shear strain intensity and the tangential stress intensity was constructed.

Let us consider standard cyclic tests in the mode of [14]: loading to $S_{\max}$ under the program $S = S_h + B(t - t_j)$ (the first stage of the cycle), exposure (usually short-term) at the maximum loading level (second stage), unloading to the initial level $S = S_h$ (third stage), heating to the temperature $T = T_{\max}$, and cooling to the initial temperature $T = T_v$ (fourth stage). Here and below, t_j are the initial and final moments of variation in the applied load and temperature.

According to (3), the microstresses can be written as $R_M = R_M^* \cos\beta \cos\lambda$ and $I_M = I_M^* \cos\beta \cos\lambda$. For an arbitrary lth cycle ($l = 0, 1, 2, \ldots$), the above-mentioned quantities at the loading stage ($j = 4l + 1$) for $B_1 = Br_1/h(T)$ have the form

$$R_M^* = r_2(S + l\Delta S); \qquad I_M^* = B_1[1 - \exp{[-h(T)(t - t_j)]} E_j],$$

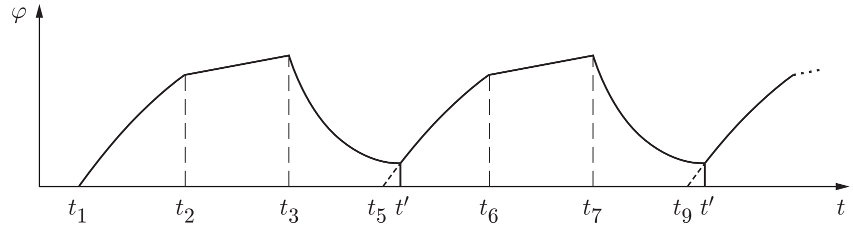

Fig. 3

where

$$\Delta S = S_{\max} - S_h,$$

$$E_j = (-1)^{H_T[4(l+1)]}\Big[\sum_{i=1}^{j-1}(-1)^{[i/2+1]}\exp\left[-h(T)(t_j - t_i)\right] + (-1)^{[j/2+1]}\Big], \qquad E_1 = 1,$$

$h(T) = \text{const}$, and $H_T(x = a)$ is the Heaviside point function.

Under the assumptions made above, the defect intensity, the irreversible-strain intensity, and the components of the irreversible-strain vector (which increases during the loading stage) are given by

$$\varphi = \Psi = a[\eta_1^{(j)}\cos^2\beta\cos^2\lambda - 1 - \eta_2^{(j)}\cos\beta\cos\lambda], \tag{6}$$

$$\varepsilon_k^p = \pi a n_k^0\{\eta_1^{(j)}[a_p(x_1)c_p(x_1) - 3(x_1)^4 b_p(x_1)/2]/3 - [a_p(x_1) - (x_1)^2 b_p(x_1)] - \eta_2^{(j)}[(x_1^2 + 1/2)\arccos x_1 - 3x_1 a_p(x_1)/2]\}.$$

Here $a_p(x) = \sqrt{1 - x^2}$, $b_p(x) = \ln|(1 + \sqrt{1 - x^2})/x|$, $c_p(x) = 1 + x^2/2$, $\eta_1^{(j)} = 3S^2/(2R^2)$, $\eta_2^{(j)} = c_1 I_M^* + c_2 R_M^*$, $R = \sigma_p(T_v)$, and x_1 is the root of the quadratic equation $\eta_1^{(j)}x_1^2 - \eta_2^{(j)}x_1 - 1 = 0$.

At the second stage of the cycle (exposure at $S = S_{\max}$), the defect intensity, the irreversible-strain intensity, and the irreversible strain at the macrolevel are defined similarly to [7]. At the third stage (unloading; we set $S_h = 0$) and fourth stage (temperature variations), there is no increment in the irreversible strain and defect relaxation occurs. Solving (1), we obtain a formula that describes the defect intensity (denoted by Ψ^*) in the period of defect relaxation:

$$\Psi^* = \Psi(t \geqslant t_{4l+3}) = [\eta_1^{(2)}\cos^2\beta\cos^2\lambda - \eta_2^{(2)}\cos\beta\cos\lambda - 1]\mathrm{e}^{-K_0(t - t_{4l+3})}. \tag{7}$$

In this case, the region of defect relaxation remains unchanged with time and corresponds to the region where $\Psi \geqslant 0$ (i.e., strain hardening occurs) during exposure at the maximum loading level. The quantity Ψ itself relaxes with time according to (7). Let, now, the next cycle begin at $t = t_{j+1}$. The defect intensity can increase; in this case (with incomplete relaxation Ψ^*) it increases from a certain non-negative value to which it relaxed in the previous cycle rather than from zero. A curve of variation in the defect intensity is shown in Fig. 3. Below, we denote by Ψ_a the defect intensity defined by (4). The moment t' at which irreversible deformation recommences is determined numerically from the relation $\Psi_a(t', \beta = 0, \lambda = 0) = \Psi^*(t', \beta = 0, \lambda = 0) = 0$. For $t \geqslant t'$, the defect intensity is described by relation (4) and the region of irreversible deformation is given by $\Psi_a(t \geqslant t') - \Psi^*(t') = 0$.

As before, the irreversible strain is determined from (6) for the corresponding values of $\eta_1^{(j)}$, $\eta_2^{(j)}$, and $\eta_3^{(j)}$. For an arbitrary number of tests, the irreversible strain is determined in a similar manner.

To validate the model, we performed calculations for Fe9%–Cr5%–Ni14%–Mn6%Si alloy specimens subjected to cyclic thermal and tensile loading according to the above scheme. The loading was varied at a high rate, the unloading in the cycle was complete ($S_h = 0$), $T_{\max} = 873$ K, and duration of exposure at $S = S_{\max}$ was equal to zero. Calculation results were compared with the experimental data of [14]. The components of the irreversible strain of defect nature were determined by the relations given above. The other components of the deformation process — the reversible martensitic strain, the elastic strain, and the thermal strain — were determined (when necessary) in accordance with [6, 7].

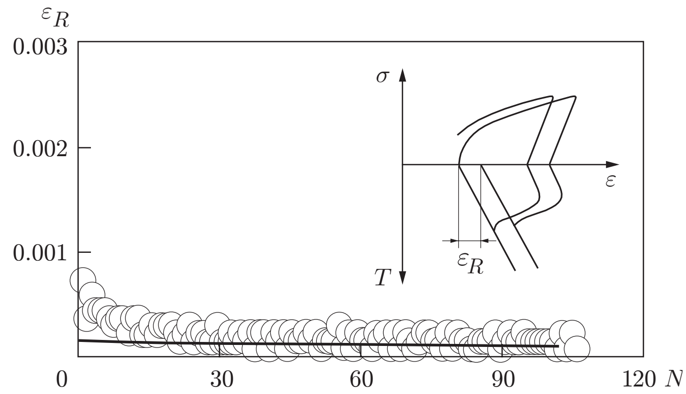

Fig. 4

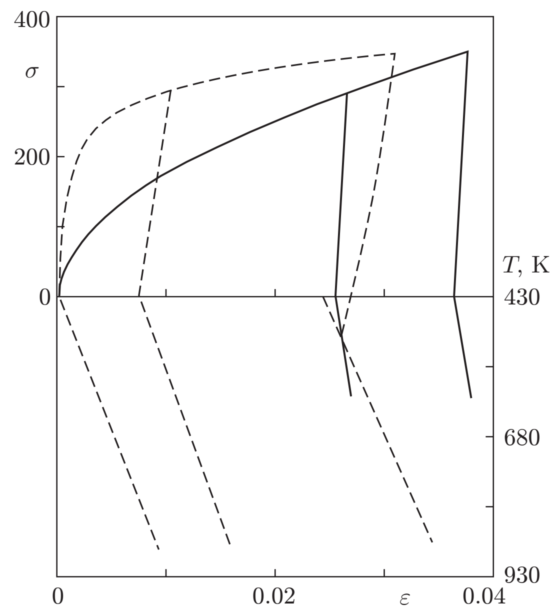

Fig. 5

Figure 4 gives the irreversible strain of dislocation nature ε_R versus the number of cycles N (the circles refer to the experimental data of [14] and the solid curves refer to the calculation result). The inset at the top of Fig. 4 shows a schematic of the variation in the total nonlinear strain during the cycle, including the relief of the reversible martensitic strain due to heating and the occurrence of the residual strain ε_R. The maximum cyclic load is $\sigma_{\max} = 350$ MPa, the exposure temperature is $T_v = 303$ K, and $T_{\max} = 873$ K. The calculation and experimental results agree quantitatively and qualitatively — the increment in the irreversible strain decreases gradually during the cycle.

Figure 5 shows the dependence of σ on ε from a double-cycle thermomechanical test according to the above-described program with a maximum load $\sigma_{\max} = 290$ MPa (first cycle) and 350 MPa (second cycle) and an exposure temperature $T_v = 430$ K. Here σ is the load applied during the cycle and ε is the total strain; the dashed curves refer to the experimental data of [14], and the solid curves refer to calculation results. The experiment shows that, at elevated exposure temperatures, the irreversible strain of defect nature is the main component of the deformation process. The martensitic strain is negligible at this exposure temperature. Thus, the theory adequately describes the deformation behavior of the specimen. The constants of the model were as follows: $K = 0.4842105$ K/MPa, $a = 4.1 \cdot 10^{-5}$, $T_{\rm con} = 340$ K, $M_s^\varsigma = 340$ K, $z_1 = 1$, $c_1 = 0$, $c_2 = 1.9$, and $r_2 = 0.05$ MPa^{-1}.

Conclusions. Among the various devices and mechanisms involving MTs, one can distinguish the wide class of so-called thermomechanical devices, in which mechanical work is performed without transforming devices (electric motors, steam generators, etc.) by converting heat to work, which is a significant advantage [15]. The material of these devices should meet the following requirements: a high level of the thermomechanical stresses developed, a high reversible strain and a minimum level of the irreversible strain induced during the MT, cyclic resistance to deterioration of the thermomechanical characteristics, reasonable cost, possibility of the two-sided shape-memory effect. Iron-based shape-memory materials meet the above requirements the most fully and, thus, they are a very important and promising materials with new properties. Owing to their characteristics, these materials can be used to design various thermomechanical devices.

The model proposed in this paper adequately describes the irreversible strain of dislocation nature for polycrystals in reversible martensitic transformations under complex thermomechanical test conditions. The model takes into account the main features of deformation processes of different natures and simultaneous manifestation of different groups of residual stresses.

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