Development of methods of structural-analytical mesomechanics that take into account the statistical properties of martensitic transformations in materials with shape memory effect

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Abstract. Methods for structural-analytical mesomechanics for materials with shape memory effect are developing, in these methods a pronounced synergetic effect is manifested, which is characterized by the appearance of self-accomodating groups of martensitic crystals, forming during the initiation of martensitic reactions extended domains oriented towards acting effective stresses.

Introduction

The calculation of the structural and mechanical behavior of polycrystals undergoing martensitic transformation under thermomechanical action is a complex task. This is due to the fact that under real deformation conditions, elements of different scale and structural levels are involved in its process, the behavior of which is determined by their individual characteristics, ensemble properties and self-consistent evolution of the structure at all interacting scale levels. A significant role is played by the statistical properties of the kinetics of martensitic phase transformations [1]. In this paper, on the basis of the results of the experimental studies carried out on thin-walled tubes of an alloy Cu–12 %Al–4 %Mn, using the methods of structural-analytical mesomechanics [2–4], we propose a model for calculating the deformation properties of materials, which takes into account the influence of the state of stress and the statistical features of phase transformations on the shape memory effects and plasticity of transformation. The model of a material with an SME can be used to solve an important problem of creating methods for calculating the stability of spherical segments of alloys with an SME under thermocyclic action [5].

1. The main hypotheses

The concentration hypothesis of the onset of martensite transformation in all structural elements of the orientation space [2] is assumed, provided that the critical nucleus of the new phase is formed. The criterion for the formation of a critical nucleus is formulated at the macroscale level in terms of effective temperature and effective stresses [1, 2] as a condition for the formation of a new phase at the macroscale level. The generalized Clausius-Clapeyron principle at the macroscale level is postulated and experimentally substantiated, which takes into account the different nature of chemical...
reactions in the forward and reverse martensitic transformation, depending on the initial phase composition. The formulation of the Clausius-Clapeyron equation uses concepts of the effective temperature \( T^* \) [2]. It is taken into account that the direct conversion of austenite to martensite (AM) occurs with the release of internal sources of heat, i.e., an exothermic reaction takes place, and in the reverse martensitic transformation of MA, an endothermic reaction occurs, that is, heat absorption in local structural elements, where the inverse reaction.

It is assumed that at the structural level self-accumulating groups of martensitic crystals arise and the plasticity of the direct martensitic transformation is determined by the disturbing effect of the deviator of local stresses [2, 6-7].

A physically grounded hypothesis is used, which asserts that the mechanism of phase reactions under the reverse martensitic transformation at the structural level obeys the "exactly backward" principle [2].

The hypothesis of an isotropic continuum at the macro-scale level and a quasicontinuum at the structural level is accepted. The influence of the anisotropy factor of martensitic crystals is reflected by taking into account the structural-static properties of the kinetics of phase transformations.

The hypotheses formulated have received good experimental substantiation both in experiments at the physical level [1] and in experimental studies on macroscale samples [2].

2. Theoretical and experimental investigation of the influence of the form of the stressed state on the thermomechanical hysteresis of the alloy Cu-12% Al-4% Mn

In materials with reversible martensitic reactions, a pronounced reversible thermomechanical hysteresis is formed during thermal cycling under voltage through the temperature range of phase transformations. An analysis of this phenomenon for simple strained states such as pure stretching and pure shear is performed within the framework of the structural-analytic theory of strength [2].

This article presents the results of a theoretical and experimental study of the influence of the form of the stressed state and the statistical properties of the kinetics of phase transformations on the thermomechanical hysteresis of an alloy Cu–12 %Al–4 %Mn.

Using the formulated hypotheses and applying the methods of structural-analytical mesomechanics for constructing models of processes of martensitic transformations and deformations initiated by them at the structural and macroscopic levels [2-8], after corresponding transformations we obtain the determining equations for the prediction of thermomechanical hysteresis in the form of formulas (1) and (2).

\[
\varepsilon_{ik}^{III} = B_h \sigma_{ik} \left( \frac{1}{2 \lambda (M_u - M_k)} \left( M_u - T + \kappa \sigma_i + \frac{\Delta}{2} \right)^2 \right) \times \left( M_u - T + \kappa \sigma_i + \frac{\Delta}{2} \right) \times H \left( T - \kappa \sigma_i - M_k - \frac{\Delta}{2} \right) \times H \left( M_u - M_k - \frac{\Delta}{2} \right) \\
+ \left( M_k - T + \kappa \sigma_i + \frac{\Delta}{2} \right) \times \left( M_u - T + \kappa \sigma_i + \frac{\Delta}{2} \right) \times H \left( M_u - T + \kappa \sigma_i - \frac{\Delta}{2} \right) \times \left( M_k - T + \kappa \sigma_i - \frac{\Delta}{2} \right) \times \left( M_u - M_k - \frac{\Delta}{2} \right) \times H \left( T - \kappa \sigma_i - M_k + \frac{\Delta}{2} \right) \times H \left( M_k - T + \kappa \sigma_i + \frac{\Delta}{2} \right) \right)
\]

(1)

Here \( \varepsilon_{ik}^{III} \) – deviation tensor of the transformation plasticity deformations, \( \sigma_{ik} \) – stress tensor deviator, \( \sigma_i \) – stress intensity, \( T \) – temperature.
To take into account statistical properties, the width of the hysteresis $\Delta$ by the following rule: $2\Delta = A_k + A_n - M_n - M_k$, where $M_n, M_k$ – characteristic temperatures of the beginning and the end under direct martensitic transformation, $A_k, A_n$ – corresponding characteristic temperatures during reverse martensitic transformation.

Equation (1), as the analysis shows, quite satisfactorily describes the kinetics of the increase in the components of the strain tensor at the cooling stage.

In the derivation of formula (2), it was assumed that the beginning of the reverse phase transition was preceded by the preliminary deformation $\varepsilon_{ik}^0$ due to the active loading of martensite or as a result of plasticity of the direct martensitic transformation, which the mathematical object stably maintained at temperature $T < M_k - \Delta/2$. Here, as the heating progressed, this deformation returned, which was classified as a shape memory effect. Calculations on details, which do not stop because of their cumbersome nature, made it possible to obtain the following general expression for the components of the tensor of restoring deformation upon heating $\varepsilon_{ik}^{\text{thr}}$:

$$
\varepsilon_{ik}^{\text{thr}} = \varepsilon_{ik}^0 \cdot H(A_k - A_n - \Delta) \cdot \left[ \frac{1}{\Delta} \left( A_n - T + \kappa \sigma_i + \frac{\Delta}{2} \right) + \frac{1}{2\Delta(A_k - A_n)} \right]
\times \left( A_k - A_n \right)^2 - \left( A_k - T + \kappa \sigma_i - \frac{\Delta}{2} \right) \cdot H \left( A_k - T + \kappa \sigma_i - \frac{\Delta}{2} \right) \cdot H \left( A_k - T + \kappa \sigma_i + \frac{\Delta}{2} \right)
+ \frac{1}{(A_k - A_n)} \left( A_k - T + \kappa \sigma_i \right) \cdot H \left( A_k - T + \kappa \sigma_i - \frac{\Delta}{2} \right) \times H \left( A_k - T + \kappa \sigma_i \right)
+ \frac{1}{2\Delta(A_k - A_n)} \left( A_k - T + \kappa \sigma_i - \frac{\Delta}{2} \right)^2 \cdot H \left( A_k - T + \kappa \sigma_i - \frac{\Delta}{2} \right) \times H \left( A_k - T + \kappa \sigma_i \right)
$$

Having experimental data on thermomechanical hysteresis, for example, in pure torsion, for two stress intensity values, it is possible to determine the model parameters that retain their values for predicting shape memory effects and plasticity of transformation for any kind of stress state.

$$
K = \frac{T_A^{\Delta \rightarrow M} - T_A^{\Delta \rightarrow M}}{\sigma_i^{(2)} - \sigma_i^{(1)}}, B_\phi = \frac{2}{3} \sigma_i^0.
$$

For alloy Cu–12%Al–4%Mn model parameters $B_\phi$ and $K$ have the following values: $B_\phi = 3,218 \times 10^6$ [MPa$^{-1}$], $K = 0,161$ [°C·MPa$^{-1}$].

Formula (2) is valid for materials with a narrow hysteresis of the phase transformation, when $\Delta = A_k - M_n \leq A_k - A_n$, which corresponds to the alloy Cu–12%Al–4%Mn. This formula leads to a rather simple and consistent with the kinetics of the recovery of deformation upon heating. It contains in the middle part of the temperature interval of mold recovery a section linear with respect to the temperature of the phase transition. At the beginning and at the end of the strain return schedule, quadratic segments with positive and negative curvature are observed, respectively.

The methods of structural-analytical mesomechanics naturally describe thermomechanical hysteresis under a complex stress state, which makes it possible to use it within the framework of solving boundary value problems of the mechanics of materials.

As an example, Picture 1 shows the results of experiments performed on thin-walled tubular samples of an alloy Cu–12%Al–4%Mn for various stress states, including a program of fifteen loading schemes, which have been described with good agreement between theoretical (solid lines) and experimental (point) results. The deviation of the theoretical data, with respect to the experimental data, does not exceed the spread (up to 5%) observed in the experiments. To calibrate the parameters of the model, it is sufficient to perform the experiment at a single stressed state, for example, under pure shear.
Picture 1. Thermomechanical hysteresis for various types of stress state. Solid lines are the results of a theoretical calculation; points are experimental data.

The stress space (a); the dependence of the strain intensity on the temperature (b); dependence of the component \( \varepsilon_{33} \) on \( T \) in points 2,3,4 (c); dependence of the component \( \varepsilon_{33} \) on \( T \) in points 7,8,9 (d); dependence of the component \( \varepsilon_{33} \) on \( T \) in points 12,13,14 (e); dependence of the component \( (2/\sqrt{3})\varepsilon_{13} \) on \( T \) in points 1,2,3,4 (f); dependence of the component \( (2/\sqrt{3})\varepsilon_{13} \) on \( T \) in points 6,7,8,9 (g); dependence of the component \( (2/\sqrt{3})\varepsilon_{13} \) on \( T \) in points 11,12,13,14 (h).
Picture 1a shows the scheme of the program for experimental and theoretical studies of thermomechanical hysteresis. The coordinates are used - the intensity of the tension at pure tension (σ), intensity of shear stress (√3τ). Circles characterize the coordinates of points of different stressed states with the same intensity of stresses σ. Three levels are considered σ = 31; 62; 93 MPa. Picture 1b shows the graphs of the thermomechanical hysteresis in the coordinates: the strain intensity εi – temperature T. Pictures 1c, d, e illustrate the kinetics of the thermomechanical hysteresis of the relative linear component of the strain tensor ε33 for various types of stress state. The graphs shown in picture 1f, g, h illustrate the thermomechanical hysteresis in the coordinates of the shear component of the strain tensor (2/√3)ε13 on temperature T. The figures in Pic.1a characterize the corresponding form of the stressed state. Comparing the obtained theoretical and experimental results, it can be noted that the proposed version of the theory makes it possible to create effective and simple methods for calculating the nontrivial deformation properties of the plasticity of transformation, shape memory, and thermomechanical hysteresis under conditions of a complex stress state in order to perform calculations of products deformed under conditions of initiation of reversible martensitic reactions.

Summing up and conclusions
Experimental studies of the processes of transformation plasticity and shape memory of an alloy Cu–12 %Al–4 %Mn in the case of a complex stressed state are fulfilled. Analytical relations at the macro-scale level in the form of equations of the deformation type (1) and (2) are obtained within the framework of structural-analytical mesomechanics methods, which is caused by the use of the concentration hypothesis and the corresponding method of integration over the variables of the microscale level of the orientation space [2]. In this case the Clausius-Clapeyron equation is formulated through the invariant of the stress tensor σ. The criterion for the formation of a critical nucleus at the structural level that triggers the martensitic reaction in all elements of the orientational space is formulated at the macro-scale level in the form of the Heaviside function operator

\[ H\left(M_n - \Phi(M_n - M_e) - T^*\right)H\left(T^*\right) = 1 \]

upon cooling during the transformation plasticity step and the operator

\[ H\left(T^* + \Phi(A_e - A_n) - A_e\right)H\left(T^*\right) = 1 \]

when heated, under conditions of initiating the effect of shape memory. The presence of the designated Heaviside operators in this model takes into account the history of thermomechanical action, which is fundamentally different from the approach of variants of deformation theory of plasticity.

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