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DEFORMATION AND FRACTURE MECHANICS

Microstructural Model for the Deformation of Shape Memory Alloys

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Abstract—A model is proposed to describe the phase-structural deformation of shape memory alloys with allowance for the nonuniform strain hardening of the martensite part of representative volume. A scheme is developed to determine the volume fraction of martensite undergoing structural transformation during proportional nonreversible loading. The problem of reactive-stress generation in experiments on orientational transformation with constrained deformation after unloading is resolved.

Keywords: shape memory alloys, phase transitions, structural transformation, nonuniform hardening, orientational transformation, reactive stresses

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INTRODUCTION

The martensite phase in a polycrystalline shape memory alloy (SMA) forms via the sequential nucleation and growth of structural constituents (lamellae or needles), which consist of martensite cells of one or several accommodated orientations. An increase in the stress intensity can cause the structural transformation of martensite, namely, the reorientation and detwining of its components [1–5]. The unique properties of SMA, such as an orientational transformation, cross hardening, and the reversing shape memory effect [1, 6], indicate different contributions of martensite components to the deformation of the representative material volume. Thus, the hardening of the martensite part of the representative SMA volume can be nonuniform.

The purpose of this work is to formulate an SMA deformation model, which takes into account the possibility of nonuniform hardening of the martensite part of the representative material volume. We also had to take into account the differences between the deformation mechanisms related to the nucleation and growth of groups of martensite components (from here on, martensite elements). Another problem was to take into account the substantial differences between the forward transformation and the martensite anelasticity diagrams of SMAs in terms of the formulated model. In addition, we tested the developed model to describe the thermomechanical loading of SMA, including the generation of reactive stresses during an orientational transformation in the constrained state.

DESCRIPTION OF THE MODEL

The results of experiments on orientational transformation [1] and the development of the strains of forward martensitic transformation under the action of decreasing stresses [6] allow us to assume that the thermoelastic phase transitions in SMA have no hardening and martensite elements can grow independently of operating stresses. On the other hand, a structural transformation causes strain hardening, which is indicated by experiments on loading specimens in the martensitic state. The stress of the beginning of the structural transformation in SMA in the martensitic state formed by cooling under a constant stress depends on this stress and usually exceeds it (cross hardening effect) [6]. Therefore, we can assume that the martensite elements having nucleated at different stresses can have different initial stresses of the beginning of a structural transformation.

In the general case of martensite formation under variable stresses and arbitrary loading of SMA, the martensite elements included in the representative volume have different hardening characteristics and undergo a structural transformation differently. The behavior of each element is described by the martensite anelasticity model proposed in [7]. This model is an analog of the theory of plastic flow, in which the maximum phase–structural strain intensity during the existence of a certain martensite element is used as an isotropic hardening parameter. Stress σ_{ij}^0 operating during the nucleation of the martensite element is assumed not to affect the law of changing the loading surface and to determine its initial state. This state is considered to correspond to the surface that forms during active loading of chaotic martensite by the stress that is proportional to σ_{ij}^0 until the structural strain intensity reaches the phase strain intensity during element nucleation. The loading surface is assumed to be unchanged during the growth and degradation of the element (during forward and reverse phase transitions, respectively).

To calculate the strain increment of the entire representative volume due to a structural transformation, we have to determine the strain increments of each martensite element. Here, the history of changing the stress with the evolution of the volume fraction of martensite is taken into account beginning from a single-phase austenitic state. The found phase–structural strain increments of the martensite elements are summed up with allowance for their volume fractions in the representative volume.

In the general case, the representative SMA volume consists of the following four parts: austenite, elastically deformable martensite elements, the martensite elements that undergo a structural transformation with purely translational hardening, and the martensite elements that undergo a structural transformation with combined hardening. The anelastic strain changes due to the structural transformation in the martensite elements with translational and combined hardening and due to phase transitions.

The tangent modulus depends on the material functions used in the analog of the theory of plasticity. When the moduli of some martensite elements are the same, their contribution to the phase-structural strain can be represented in terms of the fraction of martensite that enters in them in the representative volume. In particular, such a situation takes place during proportional loading for the martensite parts that undergo translational and (or) combined hardening. If reverse (change in the sign of stress) is absent here and austenite or chaotic martensite is the initial state of the material, no purely translational hardening occurs and the tangent modulus is identical for all elements undergoing a structural transformation.

When SMA is subjected to proportional loading, the components of the phase–structural strain and stress deviators can be expressed through parameters ε and σ, the moduli of which are equal to the strain and stress tensor intensities, respectively. The strain increment components $d\varepsilon = d\varepsilon^{\mathrm{ph}} + d\varepsilon^{\mathrm{st}}$ after forward phase transition and structural transformation and the volume fraction of martensite q can be represented as [8, 9]

$$d\varepsilon^{\mathrm{ph}} = \omega dq, \quad dq > 0; \tag{1}$$

$$q = \psi(t), \quad \psi(t) = (1 - \cos \pi t)/2, \quad dt > 0;$$

$$t = \left(M_s^0 + \omega\sigma\Delta S^{-1} - T\right)\left(M_s^0 - M_f^0\right)^{-1};$$

$$\omega = \rho_D \mathrm{sign}(\sigma)(1 - qf(q))\varphi_1(|\sigma|) + f(q)\varepsilon;$$

$$d\varepsilon^{\mathrm{st}} = G^{\mathrm{st}} d\sigma, \quad d|\sigma| > 0; \tag{2}$$

$$G^{\mathrm{st}} = q_{\mathrm{st}}\rho_D\varphi_2'(|\sigma|).$$

Here, ρ_D is the limiting phase-structural strain intensity (which correlates with the crystallographic strain intensity of the phase transformation); t is the dimensionless temperature parameter; $f(q)$ is the specific growth rate of martensite elements (no higher than $1/q$); T is the absolute temperature; M_s^0 and M_f^0 are the temperatures of the onset and end of the forward transition in the absence of stresses, respectively; ΔS is the difference between volume densities of the austenite and martensite entropies in the unloaded state at the reference temperature; and the prime in Eq. (2) designates a derivative.

The small influence of the change in the elastic moduli of SMA during the phase transition is neglected. Functions $\varphi_1(|\sigma|)$ and $\varphi_2(|\sigma|)$ increase monotonically from 0 to 1 and describe the experimental dependences of $\varepsilon_{\max}/\rho_D$ during the forward transition at a constant stress on the stress intensity and the ratio ε/ρ_D on the stress intensity during active monotonic loading of chaotic martensite.

During nonreversible proportional loading, σ does not change its sign and the modulus of ε does not decrease. In this case, martensite elements undergo a structural transformation according to a general law specified by function $\varphi_2(|\sigma|)$. The rate of changing the structural strain is expressed by Eq. (2), where the volume fraction of martensite undergoing a structural transformation at a given process point is designated as $q_{\mathrm{st}} \le q$. This rate depends on the history of martensite formation and loading.

In [8], we described a simplified algorithm for determining q_{st} for the case $\varphi_1(|\sigma|) = \varphi_2(|\sigma|)$ and $f(q) = 0$. However, the authors of [6, 10] found that an adequate description of the mechanical properties of SMA should take into account the growth of martensite elements and that the experimental dependences related to functions $\varphi_1(|\sigma|)$ and $\varphi_2(|\sigma|)$ are different. For any nonzero argument, we have $\varphi_1(|\sigma|) > \varphi_2(|\sigma|)$ [6]. Therefore, the stress of the beginning of a structural transformation σ_{tr} in a certain martensite element

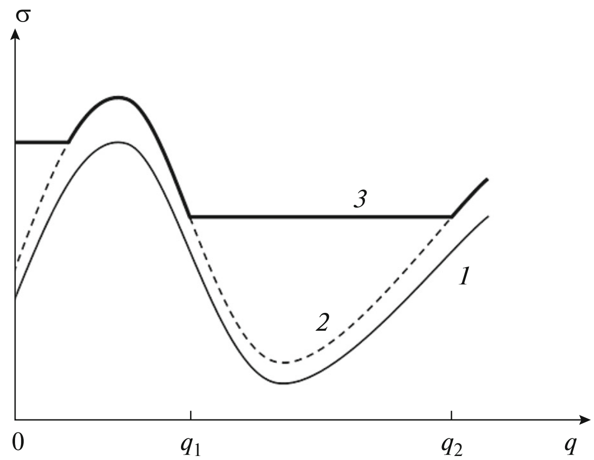

Fig. 1. Scheme for determining the part of representative volume $q_{\rm st}$ that undergoes a structural transformation.

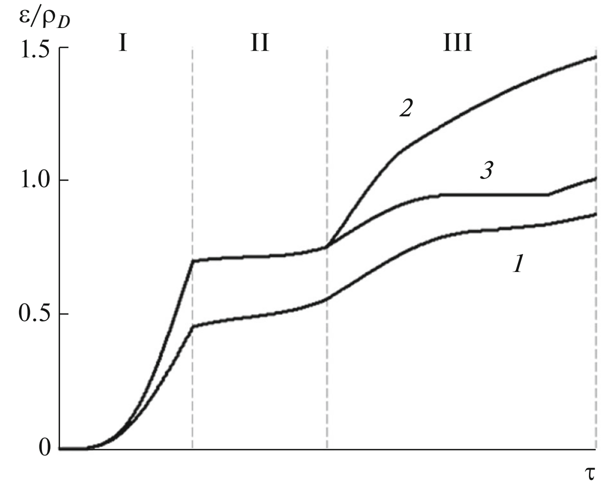

Fig. 2. Relative phase-structural strain ε/ρ_D vs. time parameter τ.

exceeds stress σ at which this element nucleated (cross hardening phenomenon),

$$\sigma_{\rm tr} = \varphi_2^{-1}\left[\varphi_1\left(|\sigma|\right)\right] > |\sigma|. \qquad (3)$$

Here, φ_2^{-1} is inverse to function $\varphi_2(|\sigma|)$.

Figure 1 shows the scheme of determining $q_{\rm st}$. It is based on the dependence of σ on q from the beginning of the forward transition to a current state (curve *1*). It can be interpreted as the stresses operating at nucleation of martensite elements on the assumption that they nucleate sequentially. This dependence was used to plot the stress of the onset of structural transformation during the nucleation of a martensite element versus q (curve *2*) and the same threshold stresses at a current point (curve *3*). The current stress corresponds to the curve *3* segment between the fractions of martensite q_1 and q_2. In this range of changing q, the martensite elements that are undergoing a structural transformation at the time under study were nucleated. Since all elements grow at specific rate $f(q)$ after nucleation, we have

$$q_{\rm st} = \bar{q}_2 - \bar{q}_1, \quad \bar{q}_k = q_k \exp\left[\int_{q_k}^{q} f(x)\,dx\right], \quad k = 1, 2. \qquad (4)$$

It should be noted that the structural transformation begins after the phase transformation.

The correctness of the model can be checked by calculating the deformation of SMA during monotonic proportional loading in an austenitic initial state (superelasticity conditions). We use the expressions

$$\varphi_1(\sigma) = \sqrt{2/\pi}\int_0^{\sigma/\sigma_0} \exp\left(-t^2/2\right)dt, \quad f(q) = (q+2)^{-1},$$

$$\varphi_2(\sigma) = 1 - \exp\left(-\sigma^2/2\sigma_0^2\right)$$

for material functions and the material parameters that are characteristic (according to experimental data) of titanium nickelide of equiatomic composition, $\sigma_0 = 150$ MPa, $M_s^0 = 332$ K, $M_f^0 = 312$ K, and $\Delta S = 406250$ J/(m^3 K).

At a constant temperature ($T = 340$ K) and an increasing stress, the relative phase-structural strain $\varepsilon/\rho_D \to 1$ in terms of the proposed model with nonuniform hardening. If the entire representative volume is involved in the structural transformation, the corresponding value tends to ($\varepsilon/\rho_D = 1.29$), i.e., the phase-structural strain intensity, is significantly higher than the limiting value.

Figure 2 shows the results of calculating the deformation of SMA under a more complex action. SMA is loaded in three stages with linear changes in stresses and temperature. At stage I, σ/σ_0 increases from 0.6 to 1.8 and temperature increases from 340 to 360 K. At stage II of the same duration, they decrease to 0.9 and 338 K, respectively. At stage III (which is twice as long), they increase to 2 and 360 K, respectively. Curve *1* corresponds to the dependence of the relative phase-structural strain ε/ρ_D on time parameter τ with allowance for nonuniform hardening, curve *2* corresponds to the case without hardening, and curve *3*, to uniform hardening.

The phase transition ends at approximately the center of stage III. Note that ε/ρ_D becomes higher than 1 when the processes described by curves *2* and *3* are completed, whereas we have $\varepsilon/\rho_D \to 1$ according to curve *1*. This discrepancy indicates the correctness of the model with nonuniform hardening. The role of martensite elements is also important. If we assume $f(q) = 0$ in the nonuniform hardening model, the phase transition stops at stage III at $\sigma = 1.8\sigma_0$ and $q = 0.6$.

If stress σ changes its sign during the forward transition in the course of proportional loading, the structural transformations of martensite elements can occur differently. The elements that did not undergo loading reverse (i.e., nucleated after the change in the sign of σ) deform according to Eq. (2), and the elements that underwent reverse deform according to another law according to a chosen analog of the theory of plasticity [7]. Then, the rate of changing the structural deformation cannot be expressed in terms of one function $\varphi_2(|\sigma|)$ and parameter q_{st}, as in Eq. (2).

PROBLEM OF THE ORIENTATIONAL TRANSFORMATION IN THE CONSTRAINED ROD

Let an SMA rod be loaded in the austenitic state by stress σ_1. Under the action of this constant stress, the rod material underwent partial forward martensitic transition to volume fraction q_1 of martensite, and the stress was then released. If further cooling occurs in a free state, phase deformation develops along the stress applied earlier (orientational transformation phenomenon) [1]. If the rod is constrained after unloading, reactive stresses of the opposite sign should develop.

At stage I, the phase transition to $q = q_1$ without the structural transformation takes place at constant stress σ_1, and we have $\varepsilon_1 = \rho_D q_1 \varphi_1(|\sigma_1|)$ at the end of the stage according to the solution to Eq. (1). The condition of predeformation after unloading at stage II is a constant total strain, which includes the deviator part of the phase-structural strain, the volume phase strain, and the elastic strain,

$$\varepsilon + \varepsilon_0 q + D(q)\sigma = \varepsilon_1 + \varepsilon_0 q_1, \qquad (5)$$

$$D(q) = \Delta D q + \frac{1}{E_A}, \quad \Delta D = \frac{1}{E_M} - \frac{1}{E_A}.$$

Here, ε_0 is the linear deformation of the volume phase transformation effect and E_M and E_A are Young's moduli of SMA in the martensitic and austenitic states, respectively.

Before stress relief, the strain is $\varepsilon_1 + \varepsilon_0 q_1 + D(q_1)\sigma_1$.

We find relation $\varepsilon(q, \sigma)$ from Eq. (5), differentiate it, set it equal to $d\varepsilon^{ph} + d\varepsilon^{st}$ according to Eq. (1), and obtain the differential equation

$$\frac{d\sigma}{dq} = -\frac{\varepsilon_0 + \Delta D\sigma + \omega(q,\sigma)}{D(q) + G^{st}(q,\sigma)}, \quad \sigma(q_1) = 0.$$

The martensite elements of the representative volume in the rod can be divided into two groups according to the stage at which they nucleate (before and after unloading). The elements having nucleated before stress relief are identically hardened because of the same stress during nucleation. At stage II, they undergo reverse loading, in contrast to the elements having nucleated after unloading (according to the calculation results, the sign of stress at the second stage remains unchanged). Therefore, the rate of changing the structural strain is

$$G^{st}(q,\sigma) = q_{st}^{1}\rho_D g'(|\sigma|) + q_{st}^{(2)}\rho_D \varphi_2'(|\sigma|),$$

where $q_{st}^{(1)}$ and $q_{st}^{(2)}$ are the volume fractions of the martensite elements that nucleated before and after unloading and undergo a structural transformation.

Function $g(\sigma)$ at low (in modulus) stresses describes a structural transformation with purely translational hardening [7]. This transformation begins simultaneously in all elements having nucleated before unloading, when stress intensity $|\sigma|$ exceeds threshold σ_1^- determined by the formula

$$\sigma_1^- = \int_0^{|\sigma_1|} \left[1 - 2\varphi_2'(x)/g'(x)\right] dx. \qquad (6)$$

When this condition is met, we have $q_{st}^{(1)} = \bar{q}_1$ according to Eq. (4); otherwise, we have $q_{st}^{(1)} = 0$. If $|\sigma|$ does not decrease after constraint (which is supported by calculations) and the condition $\varphi_1(|\sigma|) = \varphi_2(|\sigma|)$ is met, all martensite elements having nucleated after unloading are involved in the structural transformation, i.e., $q_{st}^{(2)} = q - \bar{q}_1$. If $\varphi_1(|\sigma|) \neq \varphi_2(|\sigma|)$, $q_{st}^{(2)}$ is lower than the given value and is determined at any time from a known $\sigma(q)$ dependence using the scheme shown in Fig. 1.

Figure 3 shows reactive stresses σ versus phase composition q at stage II. The calculation was performed for $\sigma_1 = 50$ MPa, $q_1 = 0.5$, and the following functions and parameters: $f(q) = (q + 2)^{-1}$, $g'(|\sigma|) = 2|\sigma|/\sigma_0$, $\varepsilon_0 = 0.001$, $\rho_D = 0.08$, $E_A = 84000$ MPa, $E_M = 28000$ MPa, and $\sigma_0 = 150$ MPa. As follows from experimental data, these parameters are characteristic of titanium nickelide.

The curves in Fig. 3a correspond to the same functions $\varphi_1(\sigma) = \varphi_2(\sigma) = 1 - \exp\left(-\sigma^2/2\sigma_0^2\right)$. Curve *1* was obtained using the proposed model with nonuniform hardening of the representative SMA volume. For comparison, we present solutions in terms of two known models [6], where Eq. (2) is used at $q_{st} = q$ under additional conditions. In the first model (curve *2*), hardening is not taken into account and an increase in stress intensity $d|\sigma| > 0$ is assumed to be a single condition for the structural transformation to occur. According to the calculations, this inequality is fulfilled after unloading and predeformation. In terms of the second model (curve *3*), hardening is uniform. For the structural transformation to occur, an increase in the stress intensity should be accompanied by the fact that this intensity is maximal over the entire history of loading from the beginning of martensite formation, $|\sigma| = |\sigma|^{max}$. Since the calculations demonstrate that $|\sigma| < |\sigma|_1$ in the constrained state, we have

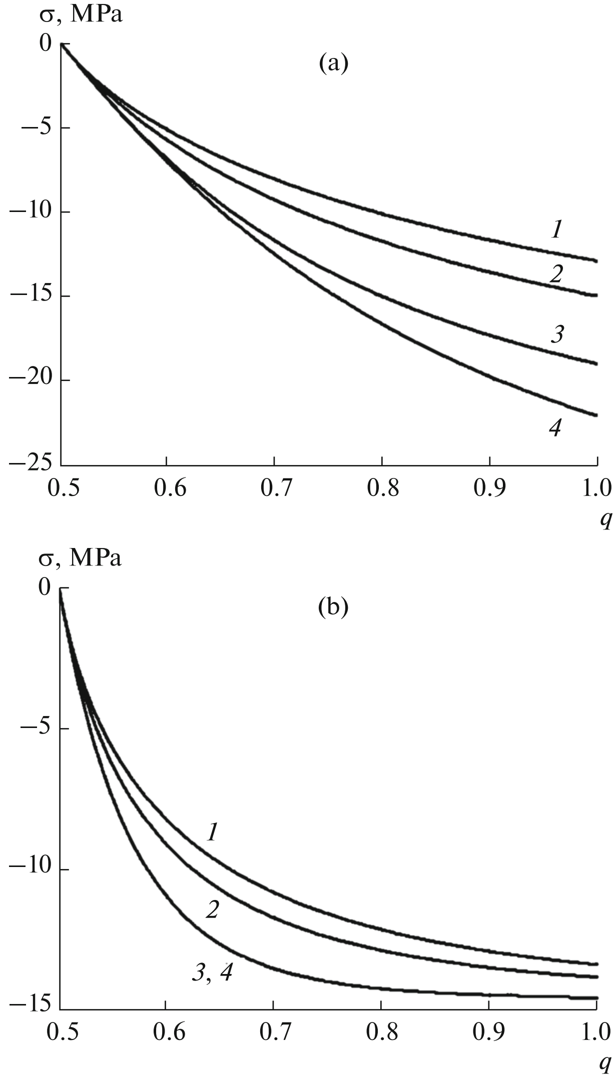

Fig. 3. Reactive stress vs. fraction of martensite: (a) $\varphi_1(|\sigma|) = \varphi_2(|\sigma|)$ and (b) $\varphi_1(|\sigma|) \neq \varphi_2(|\sigma|)$.

$q_{st} = 0$ and the structural transformation does not occur. For comparison, Fig. 3a shows the solution for another nonuniform hardening model (curve *4*). According to this model, the threshold value for the martensite elements having nucleated before unloading should be calculated using the maximum stress intensity over the entire loading history rather than Eq. (6). In this case, we have $\sigma_1^- = |\sigma_1|$ and obtain $q_{st}^{(1)} = 0$.

The curves in Fig. 3b corresponds to the functions

$$\varphi_1(\sigma) = \sqrt{2/\pi}\int_0^{\sigma/\sigma_0} \exp\left(-t^2/2\right) dt,$$

$$\varphi_2(\sigma) = 1 - \exp\left(-\sigma^2/2\sigma_0^2\right),$$

and the designations used in Fig. 3a are retained here. It should be noted that curves *3* and *4* in Fig. 3b almost coincide, since $q_{st}^{(2)}$ determined for chosen functions using the scheme presented in Fig. 1 is close to zero (at most 0.04). Therefore, the structural transformation in the martensite elements having nucleated after unloading may be neglected. The same situation takes place for the calculation by the proposed model. This finding is explained by the fact that function $\varphi_1(|\sigma|)$ has a finite derivative at zero and function $\varphi_2(|\sigma|)$ has a zero derivative. Therefore, the stress of the onset of the structural transformation σ_{tr} calculated by Eq. (3) for the element having nucleated at a low stress is substantially higher than the nucleation stress.

In terms of all models under study, the modulus of the reactive stresses increases monotonically and decelerates when the volume fraction of martensite increases. Here, the maximum modulus of the reactive stresses is multiply lower than $|\sigma_1|$. The reactive stresses depend substantially on the structural transformation model used for calculations. The suggested nonuniform hardening model gives the minimum modulus of the reactive stresses. As $|\sigma_1|$ increases, the maximum absolute value of reactive stresses increases and decelerates at high values of $|\sigma_1|$, so that this increase is very weak at $|\sigma_1| > 3\sigma_0$. It should be noted that both the orientational transformation and the volume effect of the forward phase transition contribute to the reactive stresses.

CONCLUSIONS

The proposed microstructural model for the phase-structural deformation of SMA takes into account the nonuniform hardening of representative volume and can correctly describe the thermomechanical behavior of the material. Using some examples, we showed that this model is effective for calculations, while the previously known models give contradictory results. The developed model yields the minimum modulus of the reactive stresses for the problem of orientational transformation in a constrained rod.

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