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An approach for modelling fracture of shape memory alloy parts

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Abstract. Equations describing deformation defects, damage accumulation, and fracture condition have been suggested. Analytical and numerical solutions have been obtained for defects produced by a shear in a fixed direction. Under cyclic loading the number of cycles to failure well fits the empirical Koffin-Manson law. The developed model is expanded to the case of the micro-plastic deformation, which accompanies martensite accommodation in shape memory alloys. Damage of a shape memory specimen has been calculated for two regimes of loading: a constant stress and cyclic variation of temperature across the interval of martensitic transformations, and at a constant temperature corresponding to the pseudoelastic state and cyclic variation of stress. The obtained results are in a good qualitative agreement with available experimental data.

Keywords: shape memory alloys; modeling; fracture; cyclic loading, thermocycling.

1. Introduction

Due to their special properties, shape memory alloys (SMA) are classified as functional materials, which are used as a basis for smart systems. In many practically important applications SMA parts experience cyclic variation of stress, strain and temperature. Among these applications are working bodies of martensitic engines and actuators, dampers of structure vibrations and bearings for base isolation of buildings (MANSIDE Project 1999). Thus, for efficient design of such devices, securing necessary geometric, force, time characteristics and durability one needs a model for calculation of the stress-strain state and the failure of SMA parts under loading of the mentioned types. In works (Volkov 2002, Volkov and Casciati 2001) a microstructural model has been developed describing the basic deformation effects of transformation plasticity, one-way and two-way shape memory effects and pseudoelasticity (superelasticity). At the same time, a number of phenomena have remained beyond the bounds of this model. First of all, these are damage accumulation and failure of the specimens under mechanical and thermal loading. In the present article, constitutive equations have been formulated describing the evolution of the deformation defects densities and damage produced by a plastic shear on a slip plane or by the interaction between the parent and growing martensitic phases.

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2. Defects and damage due to plastic shear on a plane

The role of deformation defects in processes of fracturing is well known, indubitable and is described in many works (see for example Friedel 1964, Hirth and Lothe 1968). Within the present approach, all deformation defects are divided in two categories: those, which are reversible and irreversible under plastic deformation. Defects of the first group are characterized by their density; for each slip plane the density is characterized by a vector $\underline{b}$, measuring the mean amount of shear on this plane. These defects may be correlated with dislocation loops expanding or shrinking under the development of the plastic deformation. They produce long-range oriented stress fields. Defects of the second type cannot move conservatively. These are split dislocations and small dislocation loops, formed by dislocation double transverse slip, bending around inclusions and incomplete annihilation. These defects “spoil” the material and produce short-range stresses. The density of the defects of the second group is denoted by f. We assume that the shear zone diameter is constant. Then, in accordance with (Popov, *et al.* 1990) one can conclude that the time derivative of the first type defect density is proportional to the plastic strain rate. This density can decrease under the plastic deformation of the opposite sign and due to the escape of the defects to the outer surface of the body. These considerations allow writing down the following equation for the evolution of the defect density $\underline{b}$ of the reversible defects

$$\dot{\underline{b}} = \dot{\underline{\beta}} - \frac{1}{\beta^*}(\underline{b}\cdot\dot{\underline{\beta}})\underline{b}^0 H(\underline{b}\cdot\dot{\underline{\beta}}) \tag{1}$$

where $\dot{\underline{\beta}}$ is plastic strain rate, $\underline{b}^0 = \underline{b}/|\underline{b}|$ – unit vector of direction $\underline{b}$, β^* – material constant and H denotes the Heaviside step function. The first term of the right side of Eq. (1) reflects the defect density changes due to formation of new defects and movement of the existing ones, while the second term - accounts for the escape of the defects to the outer surface. The density f of irreversible or scattered defects grows due to the movement of the reversible defects and it can decrease only through the thermo-activated processes of recovery with the assistance of diffusion. Taking all this into account for the defect density f one may write:

$$\dot{f} = (1 + qf)|\underline{b}||\dot{\underline{\beta}}| - r(T)f \tag{2}$$

where q, is the material constant and function $r(T)$ denotes the coefficient of the thermo-activated recovery having an Arrhenius type dependence on temperature T, that is $r(T) = r_0\exp(-U/(k_B T))$, where r_0, U are constants, k_B is Boltzmann’s constant.

To calculate the accumulation of damages, which may be identified as micro-cracks, one must formulate the micro-damage criterion. Taking into consideration that the main factor causing opening of micro-cracks is the formation of large pile-ups of the reversible defects (dislocations), which produce oriented stress fields while the scattered defects “weaken” the material thus promoting fracture, one can suggest the following condition: $|\underline{b}| = b_f/F(f)$, or

$$|\underline{b}|\cdot F(f) = b_f \tag{3}$$

where $F(f)$ is some increasing function, and b_f – the material constant, having the meaning of the critical value of the criterion $|\underline{b}|\cdot F(f)$ for creating a micro-damage.

We derive analytical solution of Eq. (1) and Eq. (2) for two cycles of the sign-alternating straining, such that the shear β occurs on one slip plane parallel (then antiparallel) to a unique direction. In this case the vector $\underline{b}$ has only one non-zero component b along this direction. For straining in one direction we find

$$b = \beta_*(1 - e^{-\beta/\beta_*})$$

$$f = \frac{1}{q}[\exp(-q\beta_*^2)\exp(q\beta_*^2(\beta/\beta_* + e^{-\beta/\beta_*})) - 1]$$

For straining in the opposite direction we have

$$b = \beta_*\left(e^{\frac{\beta-\beta_*}{\beta_*}}\left(2 - e^{-\frac{\beta_0}{\beta_*}}\right) - 1\right)$$

$$f = \frac{1}{q}\left(e^{q\beta_*^2}\exp(q\beta_*^2\left(\frac{\beta}{\beta_*} - e^{\frac{\beta_0-\beta_0}{\beta_*}}\left(2 - e^{-\frac{\beta_0}{\beta_*}}\right)\right) - 1\right) \quad (b > 0)$$

$$f = \frac{1}{q}\left(e^{q\beta_*^2}\exp(q\beta_*^2\left(e^{\frac{\beta-\beta_0}{\beta_*}}\left(2 - e^{-\frac{\beta_0}{\beta_*}}\right) - \frac{\beta}{\beta_*} + 2\left(e^{\frac{\beta_0'-\beta_0}{\beta_*}}\left(e^{-\frac{\beta_0}{\beta_*}} - 2\right) + \frac{\beta_0'}{\beta_*}\right)\right) - 1\right) \quad (b < 0)$$

where β_0' is the value of the deformation during straining in the opposite direction, at which density b changes its sign. The formulae for repeated deformation in the original direction are cumbersome and are not written here. The graphs of these dependences are shown in Fig. 1.

For simulation of the specimens deformation until failure, the function F in Eq. (3) has been taken as $F(f) = f$ or $F(f) = 1 + Af$, A being a material constant.

Modeling of the unidirectional deformation of a specimen up to its failure has shown that the fracture occurs at an ultimate value of the deformation dependent on the value of the constant b_f in Eq. (3).

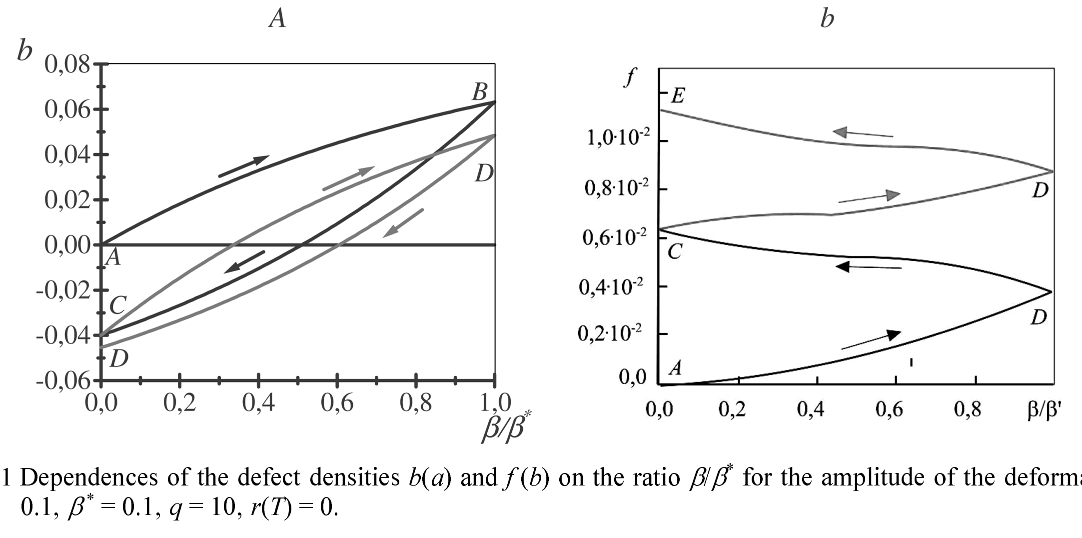

Fig. 1 Dependences of the defect densities $b(a)$ and $f(b)$ on the ratio β/β^* for the amplitude of the deformation 0.1, $\beta^* = 0.1$, $q = 10$, $r(T) = 0$.

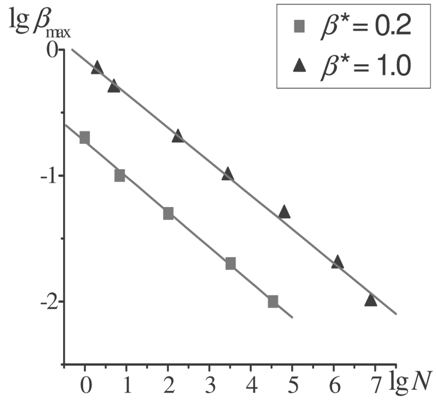

Fig. 2 Deformation amplitude β_{max} vs. number of cycles to failure N under alternating sign straining; $q = 10$, $r(T) = 0$, $F(f) = f$, $b_f = 0.1$

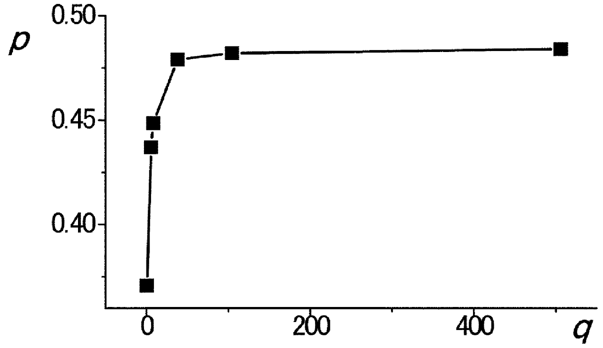

Fig. 3 Dependence of the exponent p in the Koffin – Manson law on the parameter q; $r(T) = 0$, $F(f) = f$, $b_f = 0.1$

Under alternating-sign cyclic deformation the dependence of the number of cycles to failure N on the strain amplitude β_{max} complies with the empiric Koffin – Manson power law

$$\beta_{max} \cdot N^p = M = \text{const},$$

with the exponent p dependent on the value of q (Fig. 3). One can see that in the wide range of the values of q the Manson's exponent p is close to 1/2, which is typical for many materials.

Results of the simulation has shown that the constant M depends on the constants β^*, A and b_f.

3. Defects and damage accumulation at the growth of martensite

When a martensitic crystal grows in the parent phase, internal stresses arise due to the incompatibility of the phase deformation. They may cause plastic deformation securing the accommodation of martensite. Plastic deformation takes place in the regions of the stress concentration and produces its own internal stresses opposite to the existing ones and it is these new stresses that form the two-way shape memory effect on subsequent thermocycling. This plastic deformation must also cause the multiplication of defects, damage accumulation and finally the failure of the specimen. In works (Volkov 2002, Volkov and Casciati 2001) an approach of the calculation of the microplastic deformation due to the accommodation of martensite has been developed. In particular, it was supposed that in each of the grains constituting the representative volume of the polycrystal there can arise N crystallographically equivalent variants (domain types) of martensite, and the observed microplastic deformation of a grain $\varepsilon^{gr\,MP}$ can be calculated by the formula:

$$\varepsilon^{gr\,MP} = \frac{1}{N}\sum_{n}\kappa\Phi_n^p D^{(n)} \tag{4}$$

where κ is a constant establishing the scale of the microplastic deformation, Φ_n^p are the measures of this deformation, and $D^{(n)}$ is the matrix of the deformation caused by the formation of the n-th variant of martensite. As the quantities Φ_n^p characterize the plastic deformation producing deformation defects equations, Eq. (1), Eq. (2) and the condition of the local micro-fracture Eq. (3) should be formulated for each variant of martensite:

$$\dot{b}_n = \dot{\Phi}_n^{\mathbf{p}} - \frac{1}{\beta^*}(b_n \cdot \dot{\Phi}_n^{\mathbf{p}})H(b_n \cdot \dot{\Phi}_n^{\mathbf{p}}) \tag{5}$$

$$\dot{f}_n = (1 + qf_n)|b_b||\dot{\Phi}_n^{\mathbf{p}}| - r(T)f_n \tag{6}$$

$$|b_n| \cdot F(f_n) = b_f \tag{7}$$

The conditions of macro-failure are as follows. A grain is considered fractured if condition Eq. (7) holds at least for one variant of martensite in this grain. The representative volume is considered fractured if the number of fractured grains reaches some critical value k_{cr}.

The following values of materials constants have been chosen for calculations: the characteristic temperatures of the martensitic transformation $M_s = 300$ K, $M_f = 280$ K, $A_s = 340$ K, $A_f = 360$ K, the latent heat $q_0 = -150$ MJ/m^3, the number of grains $K = 28$, other constants $\beta^* = 0.1$, $q = 0.6$, $r(T) = 0$, $b_f = 0.1$, $k_{cr} = 9$, $F(f_n) = f_n$. The cyclic life of a specimen has been studied when it was loaded by a constant stress and thermocycled through the temperature range of martensitic transformations. Comparison of the data obtained in this numerical experiment with the experimental data (Belyaev, *et al.*

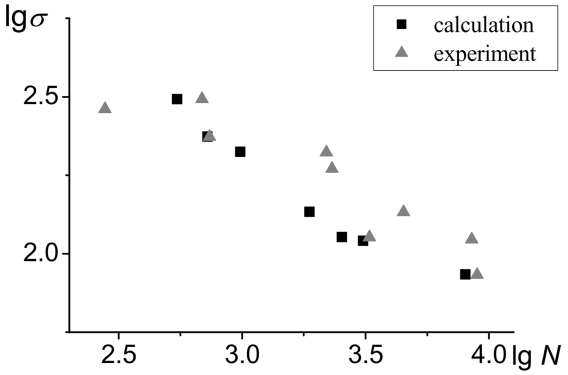

Fig. 4 Applied stress s vs. number of cycles to failure N at thermocycling of a specimen

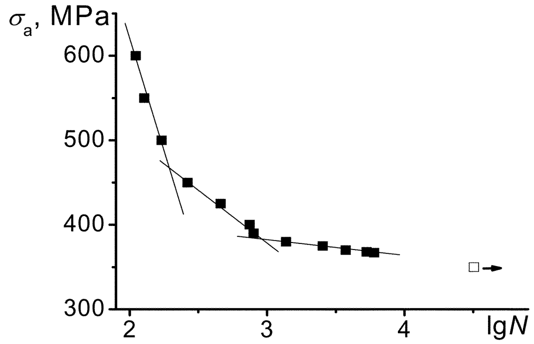

Fig. 5 Calculated dependence of the stress amplitude σ_a on the number of cycles to failure N under alternating-sign loading at 362 K

1987) (Fig. 4) shows that the developed model allows predicting the failure of a SMA specimen at thermocycles.

At alternating-sign loading in isothermal conditions at 362 K a model SMA specimen demonstrates pseudoelastic behaviour. The stress-induced growth of martensitic crystals is accompanied by a plastic accommodation causing defects and damage accumulation. Fig. 5 presents the dependence of the logarithm of the number of cycles to failure on the stress amplitude (the open square with an arrow denotes that there is no failure at this number of cycles).

These results are in qualitative agreement with experimental data (Kim and Miyazaki 1997). In particular, both the experimental and calculated dependences have three noticeable sections corresponding to three different ranges of the stress amplitude.

4. Conclusions

The developed model correctly predicts failure both under one-way and cyclic loading. In the first case failure occurs at the deformation reaching a critical value, and in the second case the number of cycles to failure complies with empiric law of Koffin-Manson. The choice of the material constants values allows obtaining different values of the ultimate strain, exponent and constant in the Koffin-Manson law.

Inclusion of the equations for the defect densities and damage evolution into the microstructural model of shape memory materials allows simulating the cyclic behaviour of the specimens both under a constant stress and temperature variations through the interval of martensitic transformations, and under alternating-sign loading in the pseudoelastic state.

The qualitative agreement of the calculated and experimental data shows that the developed model in spite of the significant simplification of the description of deformation defects and of the simplicity of the equations, nevertheless, accounts for the substantial properties of the defects and their role in fracturing.

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