

A Simple Micromechanical Model for Pseudoelastic Behavior of CuZnAl Alloy

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ABSTRACT: A simple micromechanical model for thermoelastic martensitic phase transitions (PT) is developed. It is deduced from the local description of PT in transforming particles with subsequent usage of average procedure, based on a model for elastic three-phase materials (austenite, martensite and new infinitesimal nucleus) under assumption of homogeneity of stresses in each phase. In contrast to known approaches, a new local PT criterion and a corresponding extremum principle for PT with dissipation are used. The macroscopic PT criterion obtained is split into two different equations for description of temperature-induced PT and stress-induced PT. To identify the material parameters of the model and to check its validity, simple one-dimensional experiments were carried out for CuZnAl alloy. The experimental values of martensite start and finish temperatures and austenite finish temperature for temperature-induced PT and the stress-strain diagram for stress-induced direct PT at any fixed temperature have allowed to determine six material parameters of the model for the simplest one-dimensional case. Then model prediction is compared with other independent tests. A good agreement is obtained of the calculated stress-strain curves for reverse PT (martensite-austenite) at $\theta_1 = 20^\circ\text{C}$ and for direct PT at temperature range of $30\text{--}80^\circ\text{C}$ with experimental data. Finally, the formula for determination of the transformation heat during temperature-induced PT for the given model is derived. It is shown that the predicted transformation heat is close to the experimental one.

INTRODUCTION

A number of descriptions of PT in elastic materials under one- and general three-dimensional loading based on micromechanical or phenomenological approach are known (Boyd and Lagoudas, 1996; Brinson, 1993; Leclercq and Lexcellent, 1996; Levitas and Stein, 1995, 1997; Liang and Rogers, 1990; Patoor, Eberhardt and Berveiller, 1996; Raniecki and Lexcellent, 1994; Tanaka, 1986; Sun and Hwang, 1993, and others). We will restrict ourselves to micromechanical models because we believe that it is very difficult or even impossible within a purely phenomenological approach to get expressions for transformation strain and transformation condition at multiaxial deformations. A very detailed description developed by Patoor, Eberhardt and Berveiller (1996) is very important for describing the physics, but it requires time consuming computations. An alternative approach is the formulation of a simple noncontradictory analytical three-dimensional micromechanically and thermodynamically based model. Such models can be implemented in computer codes for the analysis of structures consisting of intelligent materials. Of course these models cannot describe all details of material behavior, but this is not always necessary. For example, in plasticity theory the sim-

plest models with isotropic and kinematic hardening are the most popular for structural analysis and simulation of technological processes, despite the fact that they neglect a lot of details. The construction of such a simple model for description of shape memory alloys under complex loading is an open problem (see, e.g., Leclercq and Lexcellent, 1996). Significant progress in this direction for shape memory alloys was made by Sun and Hwang (1993). The analysis of some drawbacks of this paper is given in the paper by Levitas and Stein (1997). In papers by Levitas (see Levitas, 1997a, 1997b) a new approach for the description of PT in arbitrary dissipative materials is suggested, based on detailed thermomechanical study of small transforming regions (nucleus). Application of this approach to averaged micromechanical description of shape memory alloys is outlined in short papers by Levitas and Stein (1995, 1997), where also a comparison with results of Sun and Hwang (1993) and others is made. But detailed comparison of the developed model with experiments was not realized. It seems reasonable, before making a comparison with available two-dimensional experiments (Sittner et al., 1996; Rogueda, Lexcellent and Bocher, 1996), to check the applicability of the simplest linear variant of the model for one-dimensional tests for pseudoelastic materials.

In the second section a thermomechanical theory of PT for elastic materials with dissipation due to PT is presented. It is

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based on local consideration of small transforming volume and direct usage of the second law of thermodynamics. The theory includes a local nucleation criterion and a corresponding extremum principle. To derive the macroscopic equations for description of behavior of macrosample a model for elastic three-phase materials (austenite, martensite and new infinitesimal nucleus) is used under assumption of homogeneity of stresses in each phase (third section). The parameter, characterizing a level of internal stresses in obtained expressions for stresses in austenite (A), martensite (M) and transforming particle, is calibrated from experiments; known theoretical formulas for this parameter (Levitas, 1992; Sun and Hwang, 1993) overestimate it by one or two orders. Two different equations for description of direct PT at different levels of external stresses are obtained. The same equations—but with another value of threshold thermodynamical driving force of PT—are valid for the reverse PT. Thus, three-dimensional macroscopic model of PT was derived based on micromechanical consideration. Then simplifications of the model for uniaxial test are presented in the fourth section. Six material parameters for the model are determined from the experiments for temperature-induced PT and one experiment for direct A - M PT under tension at any fixed temperature. Then model prediction is compared with other independent tests. A good agreement of the calculated stress-strain curves for reverse PT at $\theta_1 = 20^\circ\text{C}$ and for direct PT at temperature range of 30 – 80°C with experiments is obtained. Finally the way of determination of the transformation heat during temperature-induced PT for such a model is described. It is obtained that the predicted transformation heat is close to experimental one. Some modifications of the model are discussed for future investigations.

Symbolic tensor notations are used throughout this paper. Vectors and tensors are denoted in boldface type; $\mathbf{A} \cdot \mathbf{B}$ and $\mathbf{A}:\mathbf{B}$ are contractions of tensors over one or two indices; the Euclidean norm $|\mathbf{A}| := (\mathbf{A}:\mathbf{A})^{1/2}$ is the modulus of tensor \mathbf{A} ; $:=$ means equals per definition.

THERMOMECHANICAL THEORY (LOCAL APPROACH)

Phase Transition Criterion for Elastic Materials with Dissipation Due to PT

We use the approach developed by Levitas (1997a, 1997b) for arbitrary dissipative materials. Consider a volume V of a multiphase material with prescribed boundary data on a surface S . Assume that in small volume $V_n \in V$ with the boundary Σ_n a PT occurs in time Δt (Figure 1). We apply the second law of thermodynamics for each point of a volume V_n in the form of the Planck inequality

$$\mathcal{D} = \tilde{\boldsymbol{\sigma}}:\dot{\tilde{\boldsymbol{\varepsilon}}} - \rho\dot{\psi} - \rho s\dot{\theta} \geq 0 \quad (1)$$

Here \mathcal{D} is the rate of dissipation per unit volume, ρ is the mass

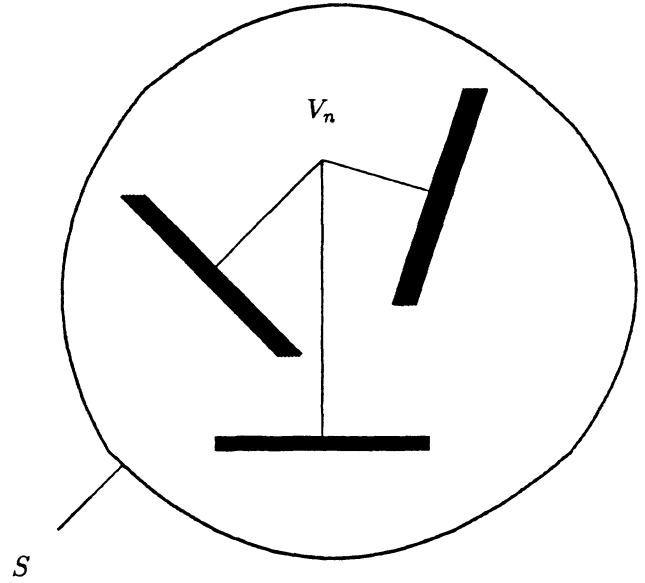


Figure 1. Multi-connected nucleus V_n inside the volume V .

density, s is the entropy, ψ is the specific Helmholtz free energy, $\tilde{\boldsymbol{\sigma}}$ and $\tilde{\boldsymbol{\varepsilon}}$ are the local (microscopic) stress and strain tensors, θ is the temperature. PT is considered as a thermomechanical process of growth of transformation (Bain) strain from the initial to the final value, which is accompanied by change of all material properties. The total dissipation increment during PT in each transforming material point is defined as

$$X := \int_1^{1+\Delta t} \mathcal{D} dt = \int_{\tilde{\boldsymbol{\varepsilon}}_1}^{\tilde{\boldsymbol{\varepsilon}}_2} \tilde{\boldsymbol{\sigma}}: d\tilde{\boldsymbol{\varepsilon}} - \Delta\psi - \int_{\theta_1}^{\theta_2} \rho s d\theta \geq 0 \quad (2)$$

where $\Delta\psi = \rho(\psi_2 - \psi_1)$, the indices 1 and 2 correspond to the value before and after PT. As we neglect all types of dissipation which are not related to PT (e.g., due to plastic flow or variation of some internal variable), the total dissipation increment coincides with the dissipation increment due to PT. At $X < 0$, PT is impossible because it contradicts the dissipative inequality. The condition $X = 0$ is the criterion for PT without dissipation due to PT because PT is possible (no contradiction to the second law of thermodynamics). Since practically all martensitic transformations, even in elastic materials, are accompanied with a dissipation and a hysteresis, the PT criterion has the form

$$X = k \quad (3)$$

Here k is an experimentally determined threshold value of dissipation due to PT (e.g., the interaction of transformation strain or moving interface with the crystal lattice defect, emission of acoustic waves, lattice friction due to Poirerls barriers, microplasticity), which can depend on some parameters, e.g., θ . At $X < k$ PT is impossible.

For each point of nucleus V_n PT criterion (3) should be ful-

filled. Integrating this criterion over the volume V_n we obtain the necessary condition of *nucleation*

$$\int_{V_n} X dV_n = \int_{V_n} k dV_n \quad (4)$$

or taking into account Equation (2) for X we get

$$\int_{V_n} \int_{\tilde{\varepsilon}_1}^{\tilde{\varepsilon}_2} \tilde{\sigma} : d\tilde{\varepsilon} dV_n - \int_{V_n} \Delta\psi dV_n + \int_{V_n} \int_{\theta_1}^{\theta_2} \rho s d\theta dV_n - \int_{V_n} k dV_n = 0 \quad (5)$$

Temperature variation in the course of PT can be determined using the first law of thermodynamics or entropy balance equation, in particular, under assumption that the process is adiabatic (Levitas, 1997b). In the following we neglect temperature variation in nucleus during PT and assume homogeneous temperature distribution.

If we decompose

$$\tilde{\varepsilon} = \tilde{\varepsilon}^e + \tilde{\varepsilon}^t \quad (6)$$

where $\tilde{\varepsilon}^e$ and $\tilde{\varepsilon}^t$ are elastic and transformation strains and assume that

$$\rho\psi_i = 0.5\tilde{\varepsilon}_i^e : \mathbf{E}_i : \tilde{\varepsilon}_i^e + \rho\psi_i^\theta, \quad i = 1, 2 \quad (7)$$

as well as $\mathbf{E}_1 = \mathbf{E}_2 = \mathbf{E}$, where \mathbf{E}_i is the tensor of elastic moduli of i -phase, ψ_i^θ is the thermal part of the free energy, then

$$\begin{aligned} \int_{\tilde{\varepsilon}_2^e}^{\tilde{\varepsilon}_1^e} \tilde{\sigma} : d\tilde{\varepsilon}^e &= \int_{\tilde{\varepsilon}_1^e}^{\tilde{\varepsilon}_2^e} \tilde{\varepsilon}^e : \mathbf{E} : d\tilde{\varepsilon}^e \\ &= 0.5(\tilde{\varepsilon}_2^e : \mathbf{E} : \tilde{\varepsilon}_2^e - \tilde{\varepsilon}_1^e : \mathbf{E} : \tilde{\varepsilon}_1^e) \end{aligned} \quad (8)$$

and it follows from Equation (5) that

$$\int_{V_n} \int_{\tilde{\varepsilon}_1^t}^{\tilde{\varepsilon}_2^t} \tilde{\sigma} : d\tilde{\varepsilon}^t dV_n - \int_{V_n} \Delta\psi^\theta dV_n - \int_{V_n} k dV_n = 0 \quad (9)$$

i.e., the elastic strains disappear.

The Postulate of Realizability

To determine all unknown parameters \mathbf{b} (position, shape and orientation of nucleus, transformation strain $\tilde{\varepsilon}^t$ and so on) the postulate of realizability is used (Levitas, 1995, 1997a, 1997b).

If starting from the state $\int_{V_n} (X(\mathbf{b}^*) - k(\mathbf{b}^*)) dV_n < 0$ for all permitted PT parameters \mathbf{b}^* (i.e., PT does not occur) in the course of continuous variation of boundary data and all possible \mathbf{b}^* condition (4) is fulfilled for the first time for some parameter \mathbf{b} , then nucleation will occur with this \mathbf{b} .

If, in the course of variation of boundary data the criterion (4) is met for one or several \mathbf{b} , then for arbitrary other \mathbf{b}^* the inequality $\int_{V_n} (X(\mathbf{b}^*) - k(\mathbf{b}^*)) dV_n < 0$ holds because PT criterion is fulfilled for the first time for parameters \mathbf{b} , but is not fulfilled for parameters \mathbf{b}^* . Consequently, we obtain the extremum principles

$$\int_{V_n} (X(\mathbf{b}^*) - k(\mathbf{b}^*)) dV_n < 0 = \int_{V_n} (X(\mathbf{b}) - k(\mathbf{b})) dV_n \quad (10)$$

for determination of all unknown parameters \mathbf{b} .

The main essence of the postulate of realizability is: if only a dissipative process (plastic flow, PT) can occur, it will occur, i.e., the first fulfillment of the necessary energetic condition is sufficient for the beginning of a dissipative process.

Note that at $k=0$ the extremum principle (10) is equivalent to the principle of minimum of Gibbs energy for the whole system (Levitas, 1997b).

PHASE TRANSITION CRITERION AND EXTREMUM PRINCIPLE FOR AVERAGED DESCRIPTION

Consider the volume V of $A + M$ mixture. During the time Δt some PT occurs in a small volume $V_n \in V$, $V_n \ll V$ with a boundary Σ (Figure 1). Volume V_n can be a multi-connected region, i.e., it can represent different martensitic variants in different grains. The following condition for the driving force X_n follows from Equation (9)

$$X_n := \frac{1}{V_n} \int_{V_n} \int_{\tilde{\varepsilon}_1}^{\tilde{\varepsilon}_2} \tilde{\sigma} : d\tilde{\varepsilon}^t dV_n - \Delta\psi^\theta = k_n \quad (11)$$

$$k_n = \frac{1}{V_n} \int_{V_n} k dV_n$$

where X_n is the dissipation increment per unit volume of V_n (driving force of PT) and k_n is the threshold value of X_n related to the actual dissipative processes in the course of PT. To get the relationship connecting local and macroscopic strains and stresses, a model for elastic three-phase materials (austenite, martensite and new infinitesimal nucleus) under the assumption of homogeneity of stresses in each phase is used (see Levitas, 1992). Under this assumption Equation (11) is equivalent to

$$X_n := \int_{\varepsilon_1}^{\varepsilon_2} \sigma_n : d\varepsilon_n^t - \Delta\psi^\theta = k_n \quad (12)$$

Here σ_n and ε_n^t are the mean stress (which equals to a local one) and transformation strain tensors in V_n . The rate of dissipation per unit volume of V due to PT is defined by $D = X_n \dot{c}_n > 0$, where $\dot{c}_n = V_n / (\Delta t V)$. In the following we will ne-

glect the volumetric transformation strain. Then from Equation (12) it follows

$$X_n = \int_{\mathbf{e}'_1}^{\mathbf{e}'_2} \mathbf{S}_n : d\mathbf{e}'_n - (\psi_2^\theta - \psi_1^\theta) = k_n \quad (13)$$

where \mathbf{S}_n and \mathbf{e}'_n are the deviators of $\boldsymbol{\sigma}_n$ and $\boldsymbol{\varepsilon}'_n$ ($= \mathbf{e}'_n$). Using the results of Levitas (1992) for a three-phase composite we obtain

$$\begin{aligned} \mathbf{S}_A &= \mathbf{S} + P\mathbf{e}^t; & \mathbf{S}_M &= \mathbf{S} - P(1-c)\mathbf{e}'_M; \\ \mathbf{S}_n &= \mathbf{S}_A - P\mathbf{e}'_n; & \mathbf{e}^t &= c\mathbf{e}'_M \end{aligned} \quad (14)$$

where \mathbf{S} and \mathbf{e}^t are the stress deviator and transformation strain averaged over the mixture (Figure 2). The subscripts A and M mean averaged over A and M values, c is the volume fraction of M , P is a parameter depending on elastic moduli. Note that $\mathbf{e}'_A \equiv 0$.

Remark 1. The consideration of three-phase composite with introduction of new infinitesimal nucleus allows us—in contrast to known approaches (for two-phase composite A and M)—to take into account in more detail the variation of the stress-strain state in transforming region.

Let us analyze expressions (14). Stresses in \mathbf{S}_A and \mathbf{S}_M consist of two parts: the external stresses \mathbf{S} and internal stresses. If $\mathbf{e}'_M = 0$, no residual stresses exist in A and M . Consequently, the internal stresses must be proportional to \mathbf{e}'_M , and P is a coefficient which transforms inelastic strain into stresses and characterizes elastic properties of a system. If there is no M , it holds $c=0$ and $\mathbf{S}_A = \mathbf{S}$; if there is no A , then $c=1$ and $\mathbf{S}_M = \mathbf{S}$. The averaged value of internal stresses over the representative volume must be zero. As $(1-c)cP\mathbf{e}'_M - c(1-c)P\mathbf{e}'_M = 0$, we fulfill this requirement. As $c_n \rightarrow 0$, the

nucleus does not affect the averaged stresses \mathbf{S}_A and \mathbf{S}_M . The expression for \mathbf{S}_n also has no qualitative contradictions. Thus, if $\mathbf{e}'_n = 0$ and the nucleus is austenitic, then $\mathbf{S}_n = \mathbf{S}_A$. If $\mathbf{e}'_n = \mathbf{e}'_M$ and the nucleus is martensitic, then

$$\mathbf{S}_n = \mathbf{S}_A - P\mathbf{e}'_M = \mathbf{S} - (1-c)P\mathbf{e}'_M = \mathbf{S}_M \quad (15)$$

Remark 2. The expression $\mathbf{S}_M = \mathbf{S}$ at $c = 1$ means that the averaged value of the residual stresses for pure martensitic state is zero. The local values of the internal stresses are in general case nonzero and their energy affects the transformation condition. If we add in the expression for X_n [Equation (12)] at the transition from the local description to the averaged one, the term which characterizes the internal stresses and is linear on the volume fraction c , then it can be formally included in the expression for k_n . The energy of the internal stresses is indirectly allowed for in the expression for the threshold value k_n that is calibrated from experiments.

There is one problem, related to the value of parameter P . Analytical expression obtained for P (Levitas, 1992) and similar expression (Sun and Hwang, 1993) yields $P \approx \mu$, where μ is a shear modulus. At $c \approx 0$ or $c \approx 1$ the maximal internal stresses \mathbf{S}_m in M or A can be estimated as

$$\mathbf{S}_m = \mu\mathbf{e}'_M = 2\mu e_Y \frac{\mathbf{e}'_M}{2e_Y} = \tau_Y \frac{\mathbf{e}'_M}{2e_Y} \quad (16)$$

where $\tau_Y = 2\mu e_Y$ and e_Y are a yield stress and an elastic strain at yielding in shear. If $e_Y \approx 10^{-3}$ for steel and $e_Y \approx 10^{-2}$ for shape memory alloys, $|\mathbf{e}'_M| \approx 10^{-1}$, then $|\mathbf{S}_m| \approx 0.5 (10 \div 100)\tau_Y$, which is impossible. The reason for the contradiction lies in the fact that simplified estimations for P do not take into account the anisotropic (plate-like) form of martensitic particles and the specific character of transformation strain distribution. For example, at transformation strain with invariant plane and formation of fine microstructure, the internal stresses are zero, but $\mathbf{e}'_M \neq 0$ (Ball and James, 1992). It is possible in principle, but extremely difficult to derive correct expression for P . That is why we shall determine the parameter P from simple experiments.

After substituting \mathbf{S}_n from Equation (14) into Equation (13) and integrating we obtain

$$\begin{aligned} X_n &= \mathbf{S}_A : (\mathbf{e}'_2 - \mathbf{e}'_1) - 0.5P(|\mathbf{e}'_2|^2 - |\mathbf{e}'_1|^2) \\ &\quad - (\psi_2^\theta - \psi_1^\theta) = k_n \end{aligned} \quad (17)$$

Under assumption of the homogeneous distribution of local stresses in nucleus the extremum principle Equation (10) can be written as

$$\begin{aligned} X_n(\mathbf{e}'_2^*, \mathbf{e}'_1^*) - k_n(\mathbf{e}'_2^*, \mathbf{e}'_1^*) &\leq 0 \\ &= X_n(\mathbf{e}'_2, \mathbf{e}'_1) - k_n(\mathbf{e}'_2, \mathbf{e}'_1) \end{aligned} \quad (18)$$

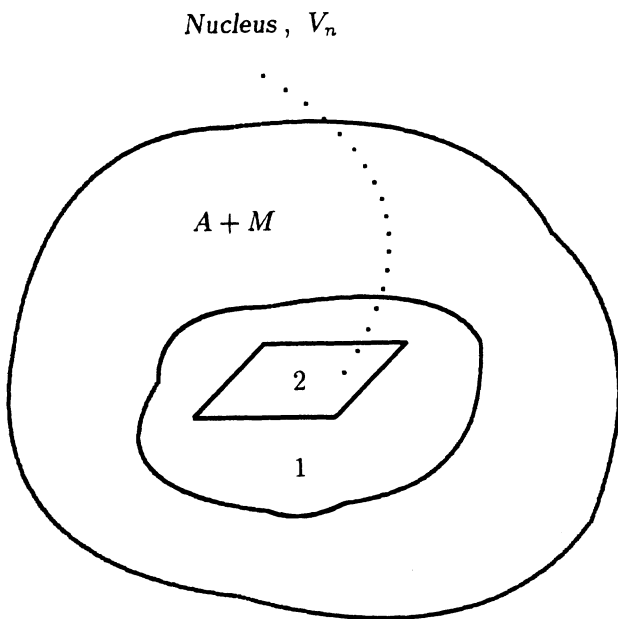


Figure 2. Scheme of averaging over volume with PT.

i.e., the real values of \mathbf{e}_i^t maximize $X_n - k_n$ in comparison with all possible \mathbf{e}_i^{t*} . Tensors \mathbf{e}_i^t meet some additional constraints, which depend on the type of PT. If k_n is independent of \mathbf{e}_i^t then from the principle (18) we obtain

$$\begin{aligned} \mathcal{S}_A : (\mathbf{e}_2^{t*} - \mathbf{e}_1^{t*}) - 0.5P(|\mathbf{e}_2^{t*}|^2 - |\mathbf{e}_1^{t*}|^2) \\ \leq \mathcal{S}_A : (\mathbf{e}_2^t - \mathbf{e}_1^t) - 0.5(|\mathbf{e}_2^t|^2 - |\mathbf{e}_1^t|^2) \end{aligned} \quad (19)$$

In a paper by Levitas and Stein (1997) five micromechanical mechanisms of PT (nucleation at direct $A \rightarrow M$ and reverse $M \rightarrow A$ PT, interface motion at direct and reverse PT and reorientation of martensitic variants) are taken into account. Here we will only consider nucleation at direct $A \rightarrow M$ and reverse $M \rightarrow A$ PT.

At direct $A \rightarrow M$ PT, $\mathbf{e}_1^t = \mathbf{e}_1^{t*} = \mathbf{e}_A^t = 0$. According to crystallography, the transformed particle consists of several variants of M in different grains. As for each variant the modulus of transformation strain equals transformation shear γ^t , and \mathbf{e}_2^t is the mean value of different variants of transformation strain over multi-connected regions of a nucleus, then $|\mathbf{e}_2^t|$ could not exceed its maximal value $a \leq \gamma^t$ which is determined from experiments. The value a can depend on c and direction $\mathbf{n} = \mathbf{e}_2^t / |\mathbf{e}_2^t|$ in transformation strain space \mathbf{e}_2^t , but in the first approximation we will neglect this dependence and consider $a = \text{const}$. Consequently it follows from the principle (19)

$$F(\mathbf{e}_2^{t*}) = \mathcal{S}_A : \mathbf{e}_2^{t*} - 0.5P|\mathbf{e}_2^{t*}|^2 \leq \mathcal{S}_A : \mathbf{e}_2^t - 0.5P|\mathbf{e}_2^t|^2 \quad (20)$$

$$\text{at } |\mathbf{e}_2^t|^2 \leq a \quad (21)$$

At $|\mathbf{e}_2^{t*}| < a$, this constraint does not affect the results, and then from condition $dF(\mathbf{e}_2^{t*})/d\mathbf{e}_2^{t*} = 0$ we obtain

$$\mathbf{e}_2^t = (1/P)\mathcal{S}_A \quad \text{at } |\mathbf{e}_2^t| < a \quad (22)$$

At $|\mathbf{e}_2^{t*}| = a$, using the method of Lagrange multiplier, we derive the following equation

$$\mathbf{e}_2^t = a\mathcal{S}_A/|\mathcal{S}_A| \quad \text{at } |\mathbf{e}_2^t| = a \quad (23)$$

Substituting Equation (22)₁ in inequality (22)₂ we obtain the constraint $|\mathcal{S}_A| < Pa$ for Equation (22)₁ in stress space. Equation (23)₁ is valid for all the values of \mathcal{S}_A in stress space because the constraint Equation (23)₂ is met in case of Equation (23)₁ for all the values of \mathcal{S}_A . Consequently at $|\mathcal{S}_A| < Pa$ both solutions Equation (22)₁ and Equation (23)₁ are possible. To choose the true solution for $|\mathcal{S}_A| < Pa$ in stress space we compared—using the extremum principle (20)—which of them maximizes X_n and obtained that for $|\mathcal{S}_A| < Pa$ the true solution is Equation (22)₁. For $|\mathcal{S}_A| \geq Pa$ only one solution, Equation

(23)₁ is valid. Substituting Equation (22)₁ and Equation (23)₁ in Equation (17) we obtain an explicit expression of $A \rightarrow M$ PT criterion in stress space

$$0.5P^{-1}|\mathcal{S}_A|^2 = (\psi_M^\theta - \psi_A^\theta) + k_{A \rightarrow M} \quad \text{at } |\mathcal{S}_A| < Pa \quad (24)$$

$$a|\mathcal{S}_A| = a^2P/2 + (\psi_M^\theta - \psi_A^\theta) + k_{A \rightarrow M} \quad \text{at } |\mathcal{S}_A| \geq Pa \quad (25)$$

Let us determine \mathbf{e}^t . By definition we have

$$\mathbf{e}^t(t) = c(t)\mathbf{e}_M^t(t) \quad \text{and} \quad (26)$$

$$\mathbf{e}^t(t + \Delta t) = c(t)\mathbf{e}_M^t(t + \Delta t) + c_n(t)\mathbf{e}_2^t(t)$$

If \mathbf{e}_M^t is not changed in previously formed $M(\mathbf{e}_M^t(t) = \mathbf{e}_M^t(t + \Delta t))$, then $\dot{\mathbf{e}}^t = \mathbf{e}_2^t \dot{c}$ and with Equations (14), (22), (23) we get

$$\frac{d\mathbf{e}^t}{dc} - \mathbf{e}^t = \frac{1}{P}\mathcal{S} \quad (27)$$

$$\mathbf{e}^t = \exp c \int_0^c \frac{1}{P}\mathcal{S}(x) \exp(-x) dx \quad \text{at } |\mathbf{e}_2^t| < a$$

$$\frac{d\mathbf{e}^t}{dc} = a \frac{\mathcal{S}_A}{|\mathcal{S}_A|} \quad \text{at } |\mathbf{e}_2^t| = a \quad (28)$$

For temperature-induced PT, $\mathcal{S} = \mathbf{0}$ and using Equations (14), (27), we get $\mathbf{e}^t = \mathcal{S}_A = \mathcal{S}_M = \mathcal{S}_n = \mathbf{e}_M^t = \mathbf{e}_2^t = \mathbf{0}$ ($|\mathbf{e}_2^t| < a$), i.e., internal stresses equal to zero for this case.

For description of a uniaxial test we will use Equation (24) for the temperature-induced PT at zero external stress and Equation (25) for the stress-induced PT. As we checked for material parameters P and a , obtained below from experiments, inequality (25)₂ is satisfied for the stress-induced PT.

At reverse $M \rightarrow A$ PT, transformation strain accumulated during $A \rightarrow M$ PT is recovered, i.e., in Equation (17) $\mathbf{e}_2^t = 0$. As $D = X_n \dot{c}_n = X_c \dot{c}$, where X_c is the dissipative force conjugated to \dot{c} and $\dot{c} = -\dot{c}_n$, it follows $X_c = -X_n$ and Equation (17) results in

$$X_c = \mathcal{S}_A : \mathbf{e}_1^t - 0.5P|\mathbf{e}_1^t|^2 - (\psi_M^\theta - \psi_A^\theta) = k_{M \rightarrow A} < 0 \quad (29)$$

where \mathbf{e}_1^t now is the transformation strain in particle of M undergoing PT. The general case of reverse PT was considered in a paper by Levitas and Stein (1997). We will use Equation (29) to model the uniaxial test.

APPLICATION OF THE MODEL FOR DESCRIPTION OF ONE-DIMENSIONAL EXPERIMENTS

Experimental Methods

At present three different types of alloying systems are used as shape memory materials: Ni-Ti-, Fe- and Cu-based alloys. For the present investigations the brass type is used. An important reason for this is the complete transformability of the high-temperature phase (austenite) into the low temperature phase (martensite). Figure 3 is evident for the complete austenite → martensite transformation of this type of alloy. This is different from Fe-based alloys where a noncomplete transformation takes place. This implies that residual austenite is left in the microstructure. Another reason for choosing a brass type alloy is the good feasibility of microstructural investigations (Different kinds of Microscopy) compared to Ni-Ti based alloys. The chemical composition as well as the transformation temperatures (M_s, M_f, A_s, A_f are the martensite start and finish temperatures and the austenite start and finish temperatures, respectively) of this alloy are given in Table 1.

The driving force for the phase transformation ($\beta \rightarrow \alpha$) can be provided by temperature changes [thermally induced martensite as shown in the micrograph (Figure 3)] or by mechanical stresses/strains. In the latter case, the martensite domains will have the orientation of the external stress tensor.

The material for the test sample was melted in a vacuum induction furnace. Sheets were produced by hot rolling at a temperature of 800°C. The material was only betatized, which implies a heat treatment at 800°C for 15 minutes and subsequently water-quenched. This treatment results in a well recrystallized material. Experiments were carried out for this nearly defect-free (exception: grain-boundaries) material. The transformation temperatures of the as betatized material were analyzed by DSC (Differential Scanning Calorimetry) measurements. Additionally, an analysis of the ther-

Table 1. Chemical composition and transformation temperatures of the investigated alloy.

| Composition | Cu | Zn | Al | |
|--------------|-------|-------|-------|-------|
| wt-% | 69.8 | 26.3 | 3.9 | |
| at-% | 66.8 | 24.4 | 8.8 | |
| Temperatures | M_f | M_s | A_s | A_f |
| °C | -35 | -8.6 | -7.1 | 5 |

mal transformation behavior ($\beta \rightarrow \alpha$) was carried out, using a light microscope with polarized light and cooling equipment.

Samples for stress tests were spark eroded from sheets (thickness: $d = 1.7$ mm). The samples (Figure 4) were polished and betatized. Prior to the stress-strain experiments the samples have undergone an age treatment at ambient temperature for 3 weeks. Stress-strain experiments were carried out with a strain rate of $\dot{\epsilon} = 0.5$ mm/min at different temperatures ($20^\circ\text{C} \leq T < 80^\circ\text{C}$). Yielding to $\epsilon = 2\%$ and subsequent unloading at a temperature of 80°C provides evidence for the fact, that no true plastic deformation due to the induction of dislocations occurs at these test conditions.

Analytical Description

Now let us simplify the equations obtained for one-dimensional tension or compression (stress-induced PT). For this case stresses and strains have the following principal components:

$$(\boldsymbol{\sigma}) = (\sigma, 0, 0), \quad (\boldsymbol{S}) = \left(\frac{2}{3}\sigma, -\frac{1}{3}\sigma, -\frac{1}{3}\sigma \right) \tag{30}$$

$$(\mathbf{e}^t) = \left(\epsilon^t, -\frac{1}{2}\epsilon^t, -\frac{1}{2}\epsilon^t \right)$$

and principal axis of \boldsymbol{S} and \mathbf{e}^t coincide. Then $|\boldsymbol{S}_A| = |\boldsymbol{S}| + P|\mathbf{e}^t|$, $\sqrt{(3/2)}|\boldsymbol{S}| = \sigma$, $\sqrt{(3/2)}\epsilon_{max}^t = |\mathbf{e}_2^t| = |\mathbf{e}_M^t| = a$, $\sqrt{(2/3)}|\mathbf{e}^t| = \epsilon^t = \epsilon_{max}^t c$, where σ , ϵ^t , ϵ_{max}^t are uniaxial stress, transformation strain and maximum value of transformation strain, respectively. Equation $\epsilon^t = \epsilon_{max}^t c$ follows from Equation (28) be-

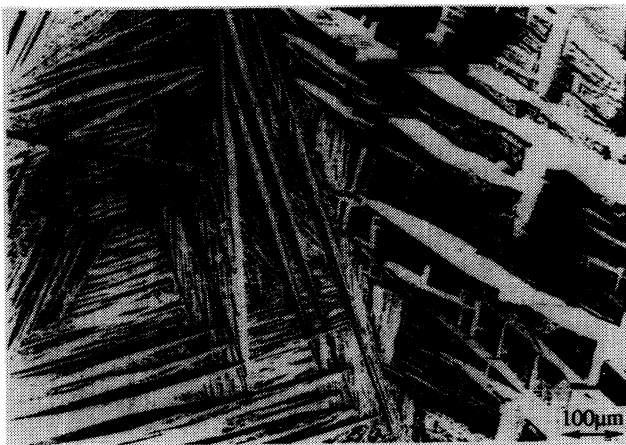


Figure 3. Thermally induced martensite. The material was betatized at 800°C for 15 min and then water quenched. LM-picture at -35°C.

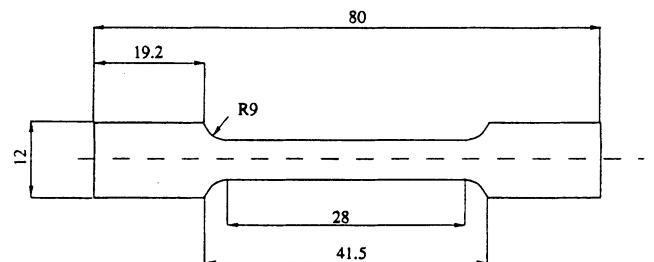


Figure 4. Sample for stress-strain experiments. The material was yielded in the as betatized condition (well recrystallized in the austenitic state).

cause $S_A/|S_A|$ is constant for uniaxial test. In our consideration we assume that Young's moduli for austenite and martensite are the same and can be determined from the initial linear part of each stress-strain diagram. Let us assume that P and a are temperature independent. The change in the thermal part of the free energy is assumed to be a linear function of θ (below we will show the validity of such approximation), i.e.,

$$\Delta\psi = \psi_M^\theta - \psi_A^\theta = \Delta\psi_0 - \Delta s_0 \theta \quad (31)$$

and

$$k_{A \rightarrow M} = b + dc, \quad k_{M \rightarrow A} = -b + d(c - 1) \quad (32)$$

are linear functions of martensite fraction c , where $\Delta\psi_0$, Δs_0 , b , d , P and a are material parameters. Then for direct austenite-martensite PT under tension or compression according to Equation (25) we have

$$X = \sigma \varepsilon'_{max} + \frac{3}{2} P (\varepsilon'_{max})^2 (c - 0.5) - \Delta\psi(\theta) = k_{A \rightarrow M}(c) \quad (33)$$

or

$$\sigma \varepsilon'_{max} + \frac{3}{2} P (\varepsilon'_{max})^2 (c - 0.5) - \Delta\psi_0 + \Delta s_0 \theta = b + dc \quad (34)$$

If, for reverse PT, we use Equation (29) at $\mathbf{e}'_1 = \mathbf{e}'_M = (\varepsilon'_{max}, -(1/2)\varepsilon'_{max}, -(1/2)\varepsilon'_{max})$ for stress-induced PT, then for reverse martensite-austenite transition the same formula for X in Equation (33) is valid, but $k_{M \rightarrow A}(c)$ should be negative

$$X = \sigma \varepsilon'_{max} + \frac{3}{2} P (\varepsilon'_{max})^2 (c - 0.5) - \Delta\psi(\theta) = k_{M \rightarrow A}(c) \quad (35)$$

or

$$\begin{aligned} \sigma \varepsilon'_{max} + \frac{3}{2} P (\varepsilon'_{max})^2 (c - 0.5) - \Delta\psi_0 + \Delta s_0 \theta \\ = -b + d(c - 1) \end{aligned} \quad (36)$$

Remark 1. Taking into account that $c = \varepsilon'/\varepsilon'_{max} = [\varepsilon - (\sigma/E)]/\varepsilon'_{max}$, where ε is total strain, E is Young's modulus, we get from Equations (34) and (36) a linear dependence between stress σ and strain ε at constant temperature for stress-induced PT.

Remark 2. For unidimensional test we could integrate Equation (28) and obtain a simple formula $c = \varepsilon'/\varepsilon'_{max}$, i.e.,

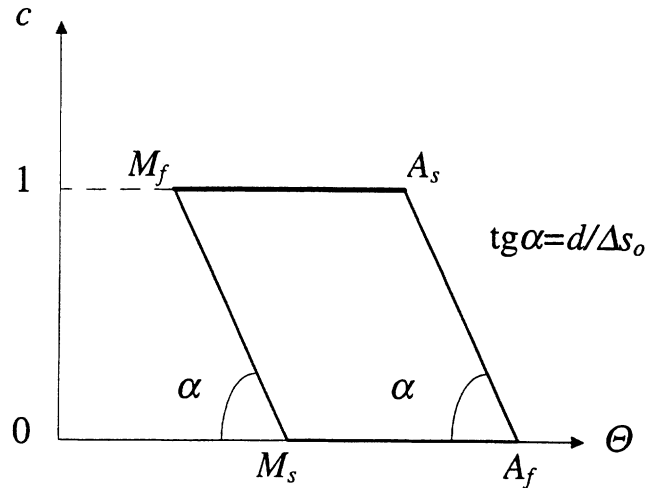


Figure 5. Volume fraction-temperature diagram for temperature-induced PT.

we could integrate kinetic equation in closed form. For multidimensional and nonproportional loading it can be more complicated.

For the case of temperature-induced PT at $S = 0$ we obtained above that $\mathbf{e}' = \mathbf{e}'_M = 0$. Then, using Equation (24), we get

$$-\Delta\psi(\theta) = k_{A \rightarrow M} \quad (37)$$

If, for reverse PT, we use Equation (29) at $\mathbf{e}'_1 = \mathbf{e}'_M = S = 0$ for temperature-induced PT, then for reverse martensite-austenite the same formula for X in Equation (37) is valid, but $k_{M \rightarrow A}(c)$ should be negative.

Thus, we get for direct PT at cooling

$$-\Delta\psi_0 + \Delta s_0 \theta = b + dc \quad (38)$$

and for reverse PT at heating

$$-\Delta\psi_0 + \Delta s_0 \theta = -b + d(c - 1) \quad (39)$$

Remark 3. The simple approximation Equations (32) accepted above means that the temperature-volume fraction diagram for temperature-induced PT forms a parallelogram [Equations (38), (39) describe two parallel lines (Figure 5)]. The case with nonparallel lines will be discussed below.

In order to use the above model for description of PT for the one-dimensional case six material parameters ε'_{max} , P , $\Delta\psi_0$, Δs_0 , b , d must be determined. It can be done, e.g., using experiments for temperature-induced PT and one experiment for direct austenite-martensite PT under tension at any fixed temperature, i.e., the unknown material parameters can be found from the following system of linear algebraic equations:

$$-\Delta\psi_0 + \Delta s_0 M_s = b \quad (40)$$

$$-\Delta\psi_0 + \Delta s_0 M_f = b + d \quad (41)$$

$$-\Delta\psi_0 + \Delta s_0 A_f = -b + d \quad (42)$$

$$\sigma_1 \varepsilon_{max}^t - \frac{3}{4} P(\varepsilon_{max}^t)^2 - \Delta\psi_0 + \Delta s_0 \theta_1 = b \quad (43)$$

$$\sigma_2 \varepsilon_{max}^t + \frac{3}{4} P(\varepsilon_{max}^t)^2 - \Delta\psi_0 + \Delta s_0 \theta_1 = b + d \quad (44)$$

Here σ_1, σ_2 are the stresses at the start of PT ($c = 0$) and at the finish of PT ($c = 1$) under tension at temperature θ_1 ; $\varepsilon_{max}^t = \varepsilon - \varepsilon^e$ is the maximum value of transformation strain at the finish of PT ($c = 1$) which equals the difference between total strain ε and elastic strains ε^e at stress σ_2 . Using experimental values of $\sigma_1 = 75$ MPa, $\sigma_2 = 131$ MPa, $\varepsilon_{max}^t = 0.02$ for direct PT at tension under $\theta_1 = 20^\circ\text{C}$ and M_s, M_f, A_f from Table 1, we solved the system of Equations (40)–(44) and defined the material parameters which are presented in Table 2. Then using the properties obtained we compared experimental data with the predicted stress-strain curves for reverse PT at $\theta_1 = 20^\circ\text{C}$ [Figure 6(a)] using Equation (36) as well as for direct PT at different temperatures (Figure 6) using Equation (34). Figures 7 and 8 show relationships for direct PT between pseudo yield stress, “hardening” modulus $d\sigma/de^t$ and temperature. The errors of results predicted by the model do not exceed spread in experimental data which is approximately equal to 15%.

Remark 4. The elastic moduli (the Young’s modulus for uniaxial test) which define the initial part of stress-strain diagram without PT in Figure 6 should be determined from experiment.

Transformation Heat during Temperature-Induced PT

Let us determine for our model an expression for transformation heat and compare it with an experiment. The energy balance equation (the first law of thermodynamics) for macroscopic representative volume reads

$$\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \rho \dot{U} - \text{div } \mathbf{h} = 0 \quad (45)$$

where U is the internal energy per unit mass, \mathbf{h} is the heat flux, div is divergence operator; per definition $\psi = U - \theta s$. For temperature-induced PT it holds $\boldsymbol{\sigma} = 0$. To calculate U let us consider two definitions of specific heat capacity of each phase at constant elastic strains (Denbing, 1981)

Table 2. Material parameters.

| | | |
|------------------------------|----------------------------|-----------------------------|
| $\varepsilon_{max}^t = 0.02$ | $\Delta\psi_0 = -13.1$ MPa | $\Delta s_0 = -0.049$ MPa/K |
| $P = 301$ MPa | $b = 0.037$ MPa | $d = 1.3$ MPa |

$$\nu_1 = \frac{\partial U_1}{\partial \theta} = \theta \frac{\partial s_1}{\partial \theta}; \quad \nu_2 = \frac{\partial U_2}{\partial \theta} = \theta \frac{\partial s_2}{\partial \theta} \quad (46)$$

Using Equation (46) and assuming that specific heat of each phase is temperature independent, we can obtain explicit expressions for the internal energy and entropy

$$U_1 = U_{10} + \nu_1(\theta - \theta_0); \quad U_2 = U_{20} + \nu_2(\theta - \theta_0) \quad (47)$$

$$s_1 = s_{10} + \nu_1 \ln \frac{\theta}{\theta_0}; \quad s_2 = s_{20} + \nu_2 \ln \frac{\theta}{\theta_0} \quad (48)$$

where s_{i0} and U_{i0} are the reference entropy and internal energy at some reference (for instance, room) temperature θ_0 .

Below we consider the case of the same specific heat $\nu = \nu_1 = \nu_2$. Then using definition $\psi_i = U_i - \theta s_i$ and Equations (47), (48) we get

$$\Delta\psi = \Delta U_0 - \theta \Delta s_0 \quad (49)$$

which we have used above for approximation of the thermal part of free energy, i.e., $\Delta\psi_0 = \Delta U_0 = U_{20} - U_{10}$, $\Delta s_0 = s_{20} - s_{10}$.

Using mixture rule for determination of internal energy of composite (because for the model developed the energy of internal stresses for temperature induced PT equal to zero)

$$U = (1 - c)U_1 + cU_2 \quad (50)$$

we get

$$\dot{U} = \Delta U_0 \dot{c} + \nu \dot{\theta} \quad (51)$$

Substituting Equation (51) in Equation (45) at $\boldsymbol{\sigma} = 0$ we have

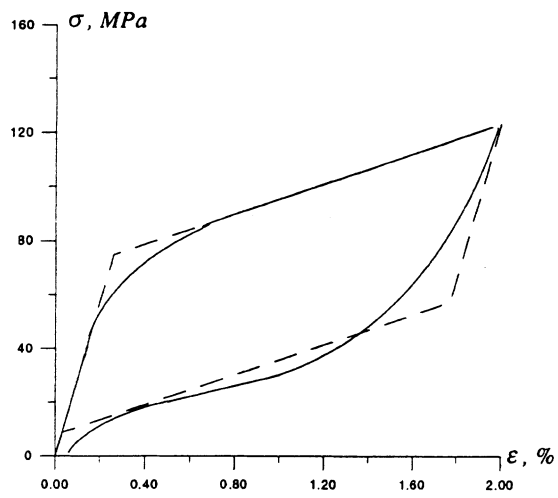
$$\nu \dot{\theta} = -\frac{1}{\rho} \text{div } \mathbf{h} - \Delta U_0 \dot{c} \quad (52)$$

where $-\Delta U_0 \dot{c}$ is the heat source, $-\int_0^1 \Delta U_0 dc = -\Delta U_0$ is the transformation heat during the whole PT. The experimental value of the transformation heat, determined by DSC, is $\Delta U_0 = -14.7$ MPa which is close to the predicted value $\Delta\psi_0$ presented in Table 2.

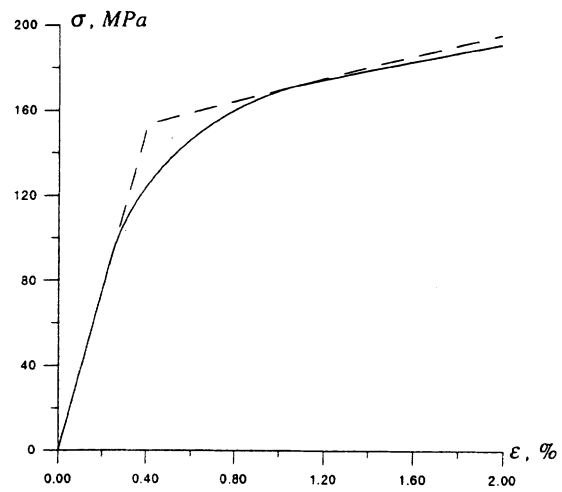
Let us consider the DSC experiment in more detail. Integrating Equation (45) over the sample volume V we get

$$Q := -\int_S \mathbf{h} \cdot \mathbf{n} dS = \int_V \rho \dot{U} dV \quad (53)$$

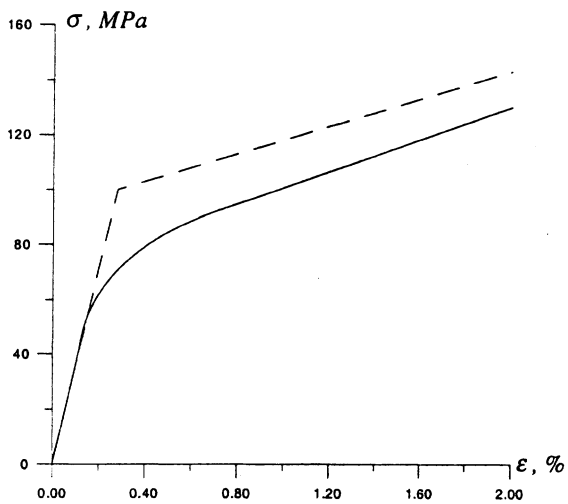
where S is the sample surface, Q is the total heat exchange rate from the sample which is measured by DSC. Using Equations (51) and (53) we obtain



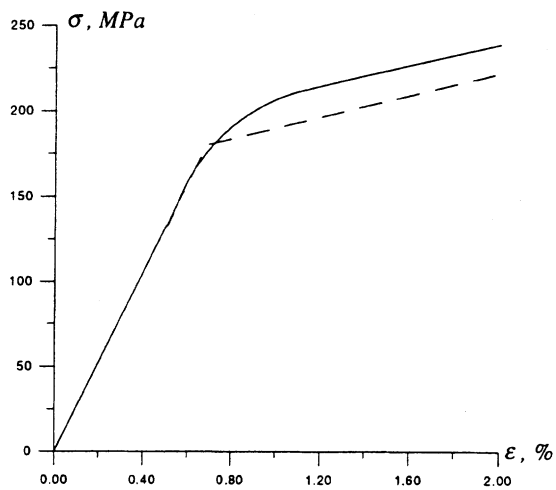
a



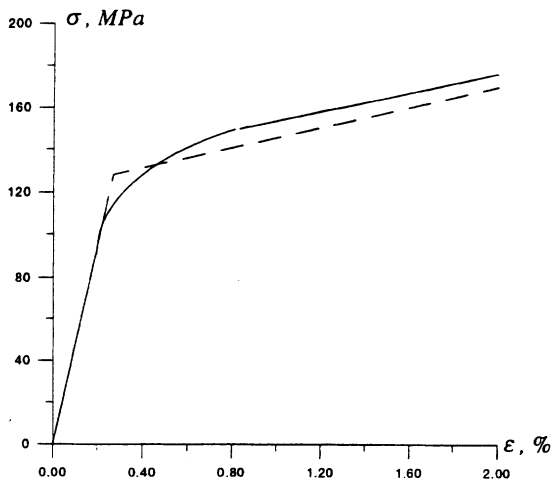
d



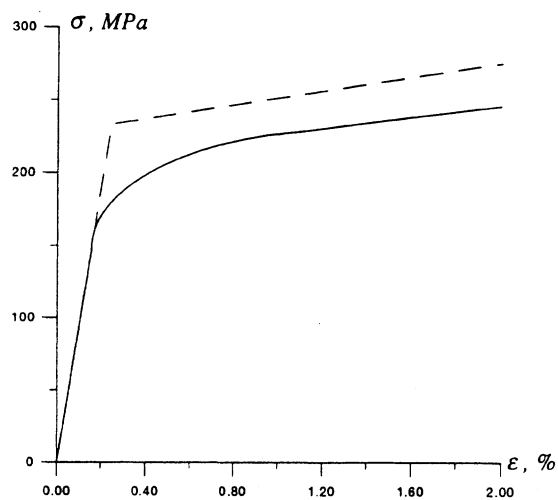
b



e



c



f

Figure 6. Stress-strain diagram at: (a) $\theta = 20^\circ\text{C}$; (b) $\theta = 30^\circ\text{C}$; (c) $\theta = 40^\circ\text{C}$; (d) $\theta = 50^\circ\text{C}$; (e) $\theta = 60^\circ\text{C}$; (f) $\theta = 80^\circ\text{C}$. — experiments, - - - results predicted by the model.

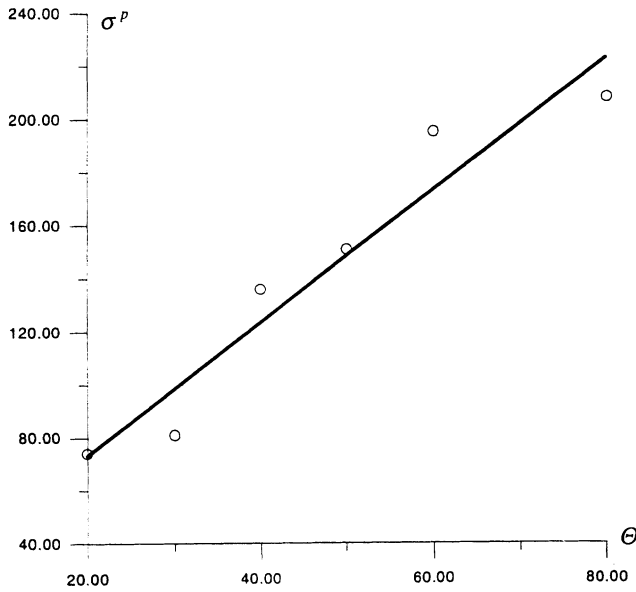


Figure 7. Relationship between pseudo yield stress σ^P and temperature θ . \circ — experiments, — — results predicted by the model.

$$m\dot{v}\theta + \Delta U_0 m \dot{c} = Q \quad (54)$$

where m is the mass of a specimen. The value $\dot{\theta} = \text{const}$ is prescribed in experiments. At cooling without PT ($\dot{c} = 0$) and measuring Q , we can determine v from Equation (54). Then measuring Q during PT we can determine from Equation (54)

$$\frac{dc}{d\theta} = \frac{Q(\theta)}{m\theta\Delta U_0} - \frac{v}{\Delta U_0} \quad (55)$$

and after integration over the temperature, we get the dependence $c(\theta)$. In particular, it follows from Equation (55) that

$$\Delta U_0 = \frac{1}{m\theta} \int_{M_s}^{M_f} Q(\theta) d\theta - v(M_f - M_s) \quad (56)$$

It is evident that the simplest linear dependence between c and θ , accepted in this paper, gives $Q(\theta) = \text{const}$ [see Equation (55)], which is not the case in experiments. For more precise model relationship between Q and c can be determined from Equation (55).

CONCLUDING REMARKS

The model developed is based on micromechanical approach with average technique and includes a new PT-criterion and the corresponding extremum principle. The final equations are rather simple, require a small number of material parameters and allow us to describe the one-dimen-

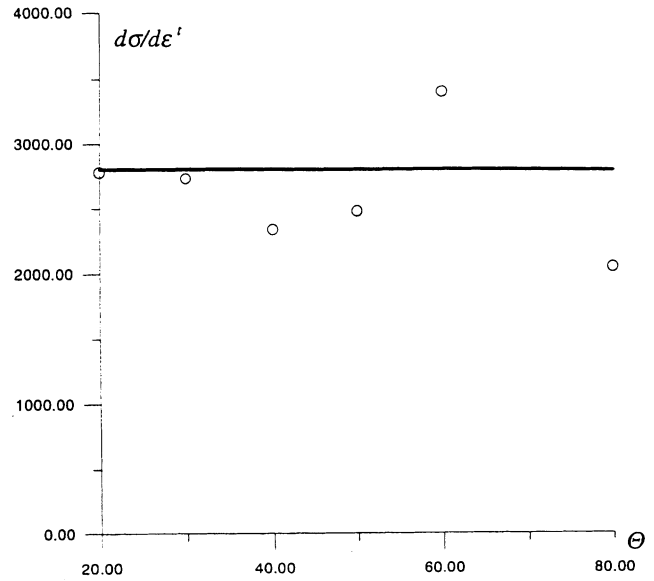


Figure 8. Relationship between coefficient $d\sigma/d\varepsilon^P$ and temperature θ . \circ — experiments, — — results predicted by the model.

sional experiments for CuZnAl alloy. But some modifications of the model should be considered in the future for description of material behavior for more complicated cases, e.g., the pseudoelastic behavior of shape memory alloys after preliminary plastic treatment (Spielfeld, Hornbogen and Franz, 1997; Treppmann and Hornbogen, 1997) and two-dimensional experiments (Sittner et al., 1996; Rogueda, LExcellent and Bocher, 1996) with proportional and nonproportional loading.

In the present model it is assumed that the difference between start and finish temperatures are the same for direct and reverse temperature-induced PT. This simplification can be taken away if we prescribe that the threshold value of driving force for reverse PT $k_{M \rightarrow A}(c) = b_r - d_r c$ has other material parameters b_r, d_r than for direct PT. The parameter d_r can be determined if we use the equation for start of reverse temperature-induced PT with temperature A_s [similar to Equations (40)–(42)]. Parameter b_r can be determined using, for example, experimental value of the transformation heat (above we used the experimental value of the transformation heat only for comparison with predicted value).

In pure martensite and for temperature-induced PT, the model predicts zero internal stresses. Such a model cannot describe the experimental situation when temperature A_s is less than equilibrium temperature θ_{eq} , determined from condition $\Delta\psi(\theta_{eq}) = 0$. In order to take into account the internal energy due to incompatibility of different martensite variants, we can assume that ψ_{02} is a growing function of c .

ACKNOWLEDGEMENT

We gratefully acknowledge the support of the Volkswagen Foundation, grant I/70283.

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