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# A MODEL FOR MEMORY ALLOYS IN PLANE STRAIN

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**Abstract**—A model for shape memory is presented which is capable of simulating the plane-strain-response of a polycrystalline body under biaxial loading. Numerical solutions to particular load histories are given.

## 1. INTRODUCTION

Memory alloys exhibit a complex stress–strain-temperature behavior which is amply documented by experimental results. Two particularly instructive books on this subject are the volumes [1, 2] which contain many experimental results and metallurgical interpretations. The basic physical reason for the occurrence of shape memory and the related effects of pseudo-elasticity are a martensitic–austenitic phase transformation and the formation of twins in the martensitic phase.

The purpose of this paper is the formulation of a model which is capable of simulating the development of the deformation of a memory alloy in plane strain, if the load and the temperature are prescribed as functions of time. The model is a natural extension of the earlier works[3, 4], but it goes beyond these on three counts:

(i) it permits biaxial loading;
(ii) it is applicable to polycrystalline bodies;
(iii) it accounts for the rotational part of a deformation.

Chapter 2 describes the model, and Chapter 3 lays down the basic equations for the description of the response of the model to time-dependent loads and temperatures. Deformation is closely linked to the phase fractions of austenite and of the martensitic twins, and creep and yield of the material are considered as thermally activated processes. Such processes are governed by rate laws for the phase fractions and by the energy equation which describes the development of temperature. To each orientation that is present in the polycrystalline body there corresponds a fraction of the austenitic and martensitic phases.

Chapter 4 relates the present theory to the general form of macroscopic constitutive equations of plastic bodies, and identifies the model as one that exhibits constitutive equations of the flow type with internal variables, viz. the phase factors.

The paper concludes with Chapter 5 in which we present solutions for uniaxial and biaxial tension and compression. The effect of rotation of the metallic lattice during the deformation is fully taken into account, but for simplicity in the numerical evaluation we consider only *one* orientation of the layers. The results show clearly the nonsymmetric stress–strain curves in tension and compression which are due to the rotation of layers. Also well exhibited is the effect of lateral loads upon the yield limit in tension and many other features that are observed in memory alloys.

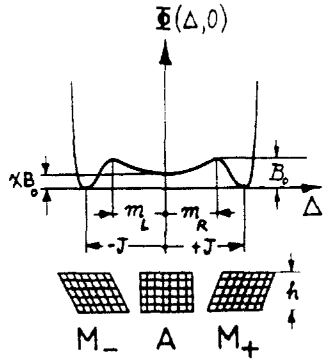


Fig. 1. Lattice particles and their potentials.

## 2. THE MODEL

### 2.1 *Basic element—lattice particle*

The basic element of the model is a lattice particle, i.e. a small piece of the metallic lattice, of which Fig. 1, in its lower part, shows three equilibrium configurations that belong to the austenitic phase $A$ and to the martensitic twins $M_+$ and $M_-$. The particles can only deform in shear, and we may take $M_\pm$ as sheared versions of $A$. The shear lengths are denoted by $\pm J$ in this case. Intermediate shear lengths $\Delta$ are also possible, and the corresponding potential energy $\Phi(\Delta)$ is assumed to have the form shown in the upper part of Fig. 1. It is composed of three different parabolae. Thus the martensitic particles may assume a stable equilibrium, while the equilibrium of the austenitic particles is metastable. The different equilibria are separated by energetic barriers at the shear lengths $m_L$ and $m_R$; $h$ is the height of a lattice particle.

If the lattice particle is subject to a shear stress $\tau$, the potential energy of the shear force, viz. $-\tau f \Delta$ must be added to $\Phi(\Delta)$. Thus the potential energy felt by lattice particles under a shear load is given by

$$\Phi(\Delta, \tau) = \Phi(\Delta) - \tau f \Delta, \tag{2.1}$$

where $f$ is the area of the upper or lower surface of the particles. This effective potential can easily be constructed by the addition of a straight line through the origin to the function $\Phi(\Delta)$ of Fig. 1. Obviously the heights of the barriers and, in general, also their position will be affected by such a shear load. Figure 2 gives a qualitative picture of the function $\Phi(\Delta, \tau)$

### 2.2 *A crystallite-stack of layers of lattice particles*

In a crystallite the lattice particles form layers, and these layers are stacked on top of each other as shown in the first picture of Fig. 3. That picture also indicates that different layers may belong to different phases, but a single layer is assumed to contain particles of only one phase. When all layers are forced into one phase, the crystallite changes its shape as shown in the second picture of Fig. 3.

The lattice particles do not lie still in the minima of the potential energy. Rather they are subject to the thermal motion so that they fluctuate about these minima. We

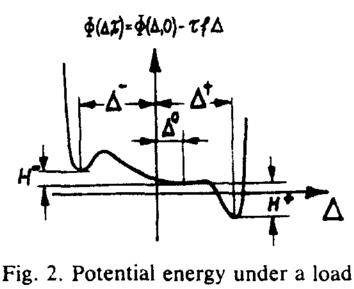


Fig. 2. Potential energy under a load.

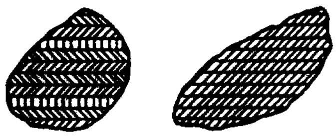

Fig. 3. Stacks of lattice layers.

call a particle austenitic or martensitic of phase $M_-$ of $M_+$, if its shear length lies in the range $(m_L, m_R)$ or $(-\infty, m_L)$, $(m_R, +\infty)$, respectively.

We can expect equilibrium to prevail within the different potential wells of the function $\Phi(\Delta, \tau)$, but the barriers between those wells may be so high that we must allow a nonequilibrium distribution of particles between the phases. In that case the tenets of statistical mechanics dictate the following probabilities for the occurrence of a particular shear length $\Delta$

$$p_\Delta^- = x^- \frac{e^{-[\Phi(\Delta,\tau)/kT]}}{\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta}; \qquad p_\Delta^0 = x^0 \frac{e^{-[\Phi(\Delta,\tau)/kT]}}{\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta};$$
$$p_\Delta^+ = x^+ \frac{e^{-[\Phi(\Delta,\tau)/kT]}}{\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta}, \qquad (2.2)$$

where $x^-$, $x^0$, $x^+$ are the fractions of particles in the phases $M_-$, $A$ and $M_+$, respectively. Also $p_\Delta^-$, $p_\Delta^0$ and $p_\Delta^+$ refer to those phases. Of course, we must have

$$x^- + x^0 + x^+ = 1. \qquad (2.3)$$

Under these circumstances the expectation value $D$ for the shear length of one layer becomes

$$D = x^- \frac{\int_{-\infty}^{m_L} \Delta\, e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta}{\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta} + x^0 \frac{\int_{m_L}^{m_R} \Delta\, e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta}{\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta}$$
$$+ x^+ \frac{\int_{m_R}^{\infty} \Delta\, e^{-[\Phi(\Phi,\tau)/kT]}\,d\Delta}{\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau)/kT]}\,d\Delta}. \qquad (2.4)$$

In (2.4) the length $D$ has been normalized so that, due to the symmetry of $\Phi(\Delta)$, $D = 0$ holds for $x^+ = x^- = 1/2$, or $x^0 = 1$ in the unloaded crystallite.

### 2.3 *A volume element—an ensemble of crystallites*

A volume element of a body is supposed to be big enough that it contains crystallites with differently oriented layers in the same proportion as those crystallites occur in the body as a whole. A schematic picture of a volume element is shown in Fig. 4.


Fig. 4. Schematic view of a volume element.

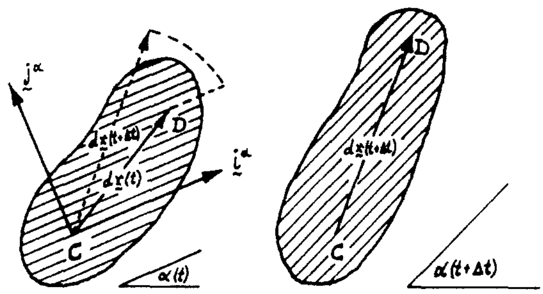


Fig. 5. Element with single orientation at times $t$ and $t + \Delta t$.

In general there may be a continuous distribution of orientations, and we write $g(\alpha, t)\,d\alpha$ for the fraction of orientations between $\alpha$ and $\alpha + d\alpha$ at time $t$. The orientation of a layer changes during a deformation and so does the distribution $g(\alpha, t)$ in general. We denote the angle of orientation in the initial or reference configuration by $A$, and $G(A)$ is the distribution in that configuration. Since $g(\alpha, t)\,d\alpha$ and $G(A)\,dA$ are fractions, we must have

$$\int_0^{\pi} g(\alpha, t)\,d\alpha = 1 \quad \text{and} \quad \int_0^{\pi} G(A)\,dA = 1. \tag{2.5}$$

Two points $C$ and $D$ in the volume element are separated by the *infinitesimal* vectors $\delta\bar{X}$, $\delta\mathbf{x}(t)$ and $\delta\mathbf{x}(t + \Delta t)$ in the reference configuration and in the configurations at time $t$ and $t + \Delta t$, respectively. We write

$$\delta\mathbf{x}(t) = \mathbf{F}(t)\delta\bar{X} \quad \text{and} \quad \delta\mathbf{x}(t + \Delta t) = \mathbf{F}(t + \Delta t)\delta\bar{X}, \tag{2.6}$$

and call $\mathbf{F}$ the deformation gradient. For simplicity we assume a plane deformation so that $F_{i3} = \delta_{i3}$ holds.

If we had only layers of orientation $\alpha$ in the element, we should calculate $\delta\mathbf{x}(t + \Delta t) - \delta\mathbf{x}(t)$, as shown in Fig. 5, as the sum of a shearing motion of the layers and of a rotation. In the frame spanned by the unit vectors $\mathbf{i}^\alpha$, $\mathbf{j}^\alpha$ along the layers and perpendicular to them respectively, the deformation could be written as

$$(D_\alpha(t + \Delta t) - D_\alpha(t))\,\frac{\delta\mathbf{x}(t)\mathbf{j}^\alpha}{h}\,\mathbf{i}^\alpha + \Delta\mathbf{Q}_\alpha\,\delta\mathbf{x}(t), \tag{2.7}$$

because $1/h\,\delta\mathbf{x}(t)\mathbf{j}^\alpha$ is the number of layers between $C$ and $D$, and $D_\alpha(t + \Delta t) - D_\alpha(t)$ is the change of the mean shear deformation of a single layer of orientation $\alpha$; the form of $D_\alpha$ is given by eqn (2.4), where the fraction $x^\pm$ and $x^0$, as well as the shear stress $\tau$, must now carry an index $\alpha$, since they may differ for different orientations. $\Delta\mathbf{Q}_\alpha$ in (2.7) is the rotational matrix.

$$\Delta\mathbf{Q}_\alpha = \begin{pmatrix} 0 & -(\alpha(t + \Delta t) - \alpha(t)) \\ \alpha(t + \Delta t) - \alpha(t) & 0 \end{pmatrix}. \tag{2.8}$$

The first picture of Fig. 5 shows the shear deformation followed by the rotation. Even if the two deformations occur simultaneously, the result is still given by eqn (2.7) to within second-order terms in $\Delta t$ and $\delta\mathbf{x}$, and this is all we shall need. All this is quite clear under the assumption that there is only one orientation.

In reality, however, the element consists of layers of many orientations, and we assume that they contribute their share eqn (2.7) to the deformation $\delta\mathbf{x}(t + \Delta t) - \delta\mathbf{x}(t)$ in the proportion $g(\alpha)\,d\alpha$ of their frequency. Thus we obtain

$$\delta\mathbf{x}(t+\Delta t) - \delta\mathbf{x}(t) = \int_0^{\pi} \left( (D_\alpha(t+\Delta t) - D_\alpha(t)) \frac{\delta\mathbf{x}(t)\cdot\mathbf{j}^\alpha}{h}\, \mathbf{i}^\alpha + \Delta\mathbf{Q}_\alpha\, \delta\mathbf{x}(t) \right) g(\alpha)\, \mathrm{d}\alpha. \quad (2.9)$$

This assumption is an important feature of the model, because it connects the macroscopically observed deformation to the shear deformation of the lattice particles and to the rotation of the lattice layers.

## 2.4 *Change of orientation during a deformation*

The construction (2.9) of the total deformation of the element as a weighted integral over the deformations of crystallites is tantamount to the view of the element as a superposition of crystallites all inflated to the size of the element, with the height of the layers augmented to $h/(g(\alpha, t)\,\mathrm{d}\alpha)$ but with $D_\alpha$ unchanged. In this manner, rare orientations contribute little to the deformation, and frequent ones contribute much and this is as it should be.

It is consistent with this view that a crystallite which has the orientation ($\cos A$, $\sin A$) in the reference configuration assumes the orientation ($\cos\alpha$, $\sin\alpha$) at time $t$, where

$$\begin{pmatrix} n\cos\alpha \\ n\sin\alpha \end{pmatrix} = \mathbf{F} \begin{pmatrix} \cos A \\ \sin A \end{pmatrix}. \quad (2.10)$$

If ($\cos A$, $\sin A$) characterizes a unit vector, $n$ is the length of that vector after the deformation.

It is thus possible to express $\alpha$ in terms of $A$, by use of the deformation gradient $\mathbf{F}$:

$$\alpha(A, t) = \arctan \frac{F_{21}\cos A + F_{22}\sin A}{F_{11}\cos A + F_{12}\sin A}, \quad (2.11)$$

or inversely

$$A(\alpha, t) = \arctan \frac{F_{11}\sin\alpha - F_{21}\cos\alpha}{F_{22}\cos\alpha - F_{12}\sin\alpha}, \quad (2.12)$$

where (2.6) has been used. Differentiation leads to

$$\frac{\partial A}{\partial\alpha} = \frac{1}{[F_{22}\cos\alpha - F_{12}\sin\alpha]^2 + [F_{11}\sin\alpha - F_{21}\cos\alpha]^2}. \quad (2.13)$$

The description of the model is completed by the trivial requirement that the number of crystallites does not change during the deformation. This requirement is expressed by the equation

$$g(\alpha, t)\,\mathrm{d}\alpha = G(A)\,\mathrm{d}A, \quad (2.14)$$

if $\alpha$ and $A$ are related by eqn (2.11) or (2.12). Usually the distribution $G(A)$ in the reference configuration will be given and eqn (2.14) may then be used to calculate $g(\alpha, t)$. By eqns (2.12) and (2.13) we obtain

$$g(\alpha, t) = G\left(\arctan \frac{F_{11}\sin\alpha - F_{21}\cos\alpha}{F_{22}\cos\alpha - F_{12}\sin\alpha}\right) \times \frac{1}{[F_{22}\cos\alpha - F_{12}\sin\alpha]^2 + [F_{11}\sin\alpha - F_{21}\cos\alpha]^2}. \quad (2.15)$$

## 3. RATE LAWS FOR DEFORMATION GRADIENT, PHASE FRACTIONS AND TEMPERATURE

### 3.1 *Deformation gradient*

3.1.1 *Rate law for deformation gradient.* By (2.6) we may replace $\delta\mathbf{x}(t)$ by $\mathbf{F}(t)\delta\bar{X}$, and $\delta\mathbf{x}(t + \Delta t)$ by $\mathbf{F}(t + \Delta t)\delta\bar{X}$, and thus the difference equation (2.9) becomes a rate law for $\dot{\mathbf{F}}$, if we let $\Delta t$ tend to zero. We obtain

$$\dot{F}_{ij} = \int_0^\pi g(\alpha, t)\left[\frac{1}{h}\dot{D}_\alpha i_i^\alpha j_k^\alpha + \begin{pmatrix} 0 & -\dot{\alpha} \\ \dot{\alpha} & 0 \end{pmatrix}_{ik}\right] F_{kj}\, \mathrm{d}\alpha, \tag{3.1}$$

or more explicitly, if the components of the unit vectors $\mathbf{i}^\alpha$ and $\mathbf{j}^\alpha$ are introduced,

$$\dot{F}_{ij} = \int_0^\pi g(\alpha, t)\begin{bmatrix} -\frac{1}{h}\dot{D}_\alpha \sin\alpha\cos\alpha & \frac{1}{h}\dot{D}_\alpha \cos^2\alpha - \dot{\alpha} \\ -\frac{1}{h}\dot{D}_\alpha \sin^2\alpha + \dot{\alpha} & \frac{1}{h}\dot{D}_\alpha \sin\alpha\cos\alpha \end{bmatrix} F_{kj}\, \mathrm{d}\alpha. \tag{3.2}$$

It is useful to define the abbreviations

$$I^{ss}(\dot{D}) = \int_0^\pi g(\alpha, t)\frac{1}{h}\dot{D}_\alpha \sin^2\alpha\, \mathrm{d}\alpha, \qquad I^{sc}(\dot{D}) = \int_0^\pi g(\alpha, t)\frac{1}{h}\dot{D}_\alpha \sin\alpha\cos\alpha\, \mathrm{d}\alpha,$$

$$I^{cc}(\dot{D}) = \int_0^\pi g(\alpha, t)\frac{1}{h}\dot{D}_\alpha \cos^2\alpha\, \mathrm{d}\alpha, \qquad I = \int_0^\pi g(\alpha, t)\dot{\alpha}\, \mathrm{d}\alpha, \tag{3.3}$$

because in this manner the eqns (3.2) may be written in an abbreviated form as follows:

$$\begin{array}{llllll}
\dot{F}_{11} = & -I^{sc}(\dot{D})F_{11} & & (I^{cc}(\dot{D}) - I)F_{21} & \\
\dot{F}_{12} = & & -I^{sc}(\dot{D})F_{12} & & (I^{cc}(\dot{D}) - I)F_{22} \\
\dot{F}_{21} = & (-I^{ss}(\dot{D}) + I)F_{11} & & I^{sc}(\dot{D})F_{21} & \\
\dot{F}_{22} = & & (-I^{ss}(\dot{D}) + I)F_{12} & & I^{sc}(\dot{D})F_{22}
\end{array} \tag{3.4}$$

From these formulae it may be confirmed by direct calculation that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\det \mathbf{F}) = \dot{F}_{11}F_{22} + F_{11}\dot{F}_{22} - \dot{F}_{12}F_{21} - F_{12}\dot{F}_{21} = 0 \tag{3.5}$$

holds, so that the possible deformations of the model are isochoric. This is proper, since the deformation is a superposition of simple shearing and rotation. Integration of eqn (3.5) leads to

$$\det \mathbf{F} = 1, \tag{3.6}$$

since initially we have

$$\mathbf{F} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

The eqns (3.4) seem to be linear equations in $\mathbf{F}$, but a closer investigation reveals many nonlinearities, because the integrals $I$ depend on $\mathbf{F}$, and $\dot{\mathbf{F}}$, in several ways. Indeed, by eqn (2.15), the distribution $g(\alpha, t)$ is a function of $\mathbf{F}$. Also $\dot{\alpha}$, by eqn (2.11), depends on $\mathbf{F}$ and $\dot{\mathbf{F}}$, and $\dot{D}_\alpha$ is a function of many variables; among them $\mathbf{F}$ and $\dot{\alpha}$. We proceed to list these dependencies.

3.1.2 *Dependence of the integrals* I *on* $\mathbf{F}$. The dependence of $\dot{\alpha}$ on $\alpha$, $\mathbf{F}$ and $\dot{\mathbf{F}}$ follows from eqn (2.11) by differentiation and subsequent elimination of $A$ by use of eqn (2.12). The resulting formula is too complicated to be listed here, but it is quite explicit. For later reference, we merely write

$$\dot{\alpha} = \frac{\partial \alpha}{\partial F_{ij}} \dot{F}_{ij} = A(\alpha, \mathbf{F}, \dot{\mathbf{F}}). \tag{3.7}$$

The dependence of $\dot{\alpha}$ upon the components of $\dot{\mathbf{F}}$ is obviously linear.

It remains to calculate $\dot{D}_\alpha$, which occurs in most of the integrals $I$ defined by eqn (3.13). We recall the form (2.4) of the expected shear length which must be modified, as stated before, by attaching indices $\alpha$ to $x^{\pm}$, $x^0$ and $\tau$. The relation of the shear stress $\tau_\alpha$ to the externally applied stress tensor $\boldsymbol{\sigma}$ may be read off from the well-known Mohr circle, and we have

$$\tau_\alpha = \sigma_{ij}\, i_i^\alpha j_j^\alpha = \frac{\sigma_{22} - \sigma_{11}}{2} \sin 2\alpha + \sigma_{12} \cos 2\alpha. \tag{3.8}$$

$\dot{D}_\alpha$ can now be obtained by differentiation of $D_\alpha$ in eqn (2.4). This is quite an easy task but, here again, the result is too long to be written down. Instead we present only the general structure of that expression, and write

$$\dot{D}_\alpha = K_\alpha \left( \frac{\partial \tau_\alpha}{\partial \alpha} \dot{\alpha} + \frac{\partial \tau_\alpha}{\partial \sigma_{ij}} \dot{\sigma}_{ij} \right) + S_\alpha \dot{T} + X_\alpha^- \dot{x}_\alpha^- + X_\alpha^0 \dot{x}_\alpha^0 + X_\alpha^+ \dot{x}_\alpha^+ , \tag{3.9}$$

where the coefficients $X_\alpha^{\pm}$ and $X_\alpha^0$ are given by

$$X_\alpha^- = \frac{\int_{-\infty}^{m_L} \Delta\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}{\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}, \qquad X_\alpha^0 = \frac{\int_{m_L}^{m_R} \Delta\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}{\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta},$$

$$X_\alpha^+ = \frac{\int_{m_R}^{\infty} \Delta\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}{\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}, \tag{3.10}$$

as can be read off from eqn (2.4). The coefficients $K_\alpha$ and $S_\alpha$ are defined as

$$K_\alpha \equiv \frac{\partial D_\alpha}{\partial \tau_\alpha}$$

or, by (2.4),

$$K_\alpha = f \frac{1}{kT} \left\{ x_\alpha^- \frac{\left( \int_{-\infty}^{m_L} \Delta^2 e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta \right) \left( \int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta \right) - \left( \int_{-\infty}^{m_L} \Delta\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta \right)^2}{\left( \int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta \right)^2} \right.$$

$$+ x_\alpha^0 \frac{\left(\int_{m_L}^{m_R} \Delta^2 \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right) - \left(\int_{m_L}^{m_R} \Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)^2}{\left(\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)^2}$$

$$\left. + x_\alpha^+ \frac{\left(\int_{m_R}^{\infty} \Delta^2 \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right) - \left(\int_{m_R}^{\infty} \Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)^2}{\left(\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)^2} \right\} \tag{3.11}$$

$$S_\alpha \equiv \frac{\partial D_\alpha}{\partial T}$$

or, by eqn (2.4),

$$S_\alpha = \frac{1}{kT^2} \left\{ x_\alpha^- \frac{\left(\int_{-\infty}^{m_L} \Phi(\Delta, \tau_\alpha)\Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right) - \left(\int_{-\infty}^{m_L} \Phi(\Delta, \tau_\alpha) \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{-\infty}^{m_L} \Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)}{\left(\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)^2} \right.$$

$$+ x_\alpha^0 \frac{\left(\int_{m_L}^{m_R} \Phi(\Delta, \tau_\alpha)\Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right) - \left(\int_{m_L}^{m_R} \Phi(\Delta, \tau_\alpha) \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{m_L}^{m_R} \Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)}{\left(\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)^2}$$

$$\left. + x_\alpha^+ \frac{\left(\int_{m_R}^{\infty} \Phi(\Delta, \tau_\alpha)\Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right) - \left(\int_{m_R}^{\infty} \Phi(\Delta, \tau_\alpha) \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)\left(\int_{m_R}^{\infty} \Delta \, e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)}{\left(\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]} \, d\Delta\right)^2} \right\} \tag{3.12}$$

The derivatives $\partial\tau_\alpha/\partial\alpha$ and $[\partial\tau_\alpha/\partial\sigma_{ij}]\,\dot{\sigma}_{ij}$ follow from eqn (3.8), and we have

$$\frac{\partial\tau_\alpha}{\partial\alpha} = (\sigma_{22} - \sigma_{11}) \cos 2\alpha - \sigma_{12} \sin 2\alpha, \tag{3.13}$$

$$\frac{\partial\tau_\alpha}{\partial\sigma_{ij}} \dot{\sigma}_{ij} = \frac{\dot{\sigma}_{22} - \dot{\sigma}_{11}}{2} \sin 2\alpha + 2\dot{\sigma}_{12} \cos 2\alpha. \tag{3.14}$$

All five coefficients in eqn (3.9) are functions of $\boldsymbol{\sigma}$, $T$ and $\alpha$, and $K_\alpha$, $S_\alpha$ depend on $x_\alpha^\mp$ and $x_\alpha^0$ in addition.

3.1.3 *Summary.* The right-hand side of eqn (3.9) is a function of the variables

$$\mathbf{F},\ \dot{\mathbf{F}},\ \boldsymbol{\sigma},\ \dot{\boldsymbol{\sigma}},\ T,\ \dot{T},\ x_\alpha^\mp,\ x_\alpha^0,\ \dot{x}^\mp,\ \dot{x}^0 \tag{3.15}$$

whose form can be calculated once $\Phi(\Delta)$ is given. It can also be seen that the rates occuring among the quantities in eqn (3.15) appear linearly in $\dot{D}_\alpha$ and $\dot{\alpha}$. Therefore the integrals in eqn (3.3) also depend linearly on $\dot{\mathbf{F}}$, $\dot{\boldsymbol{\sigma}}$, $\dot{T}$, $\dot{x}_\alpha^\mp$, $\dot{x}_\alpha^0$.

Insertion of the integrals $I$ into the rate laws (3.4) will thus produce a system of equations, in which $\dot{\mathbf{F}}$ is related to the given external loading $\boldsymbol{\sigma}(t)$. However, that relation is effected by the functions $T(t)$ and $x_\alpha^\mp(t)$, $x_\alpha^0(t)$, which themselves must still be determiined.

We proceed to formulate the rate laws that govern the behavior of the phase fractions $x$ and of temperature.

### 3.2 *Phase fractions*

The equations for the evolution of the phase fractions are based on the idea that the transition probability of a lattice particle across the barriers of the potential energy at $m_L$ and $m_R$ are proportional to the probability of finding the particle at the height of the barrier and moving in the right direction. The expressions for the transition probabilities $p_\alpha^{-0}$, $p_\alpha^{0-}$, $p_\alpha^{0+}$ and $p_\alpha^{+0}$ that result from this idea have been derived in [6], and here we only list the results:

$$p_\alpha^{-0} = k_l\sqrt{\frac{kT}{2\pi m}}\,\frac{e^{-[\Phi(m_L,\tau_\alpha)/kT]}}{\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,d\Delta}, \qquad p_\alpha^{0-} = k_c\sqrt{\frac{kT}{2\pi m}}\,\frac{e^{-[\Phi(m_L,\tau_\alpha)/kT]}}{\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,d\Delta}, \tag{3.16$_1$}$$

$$p_\alpha^{0+} = k_c\sqrt{\frac{kT}{2\pi m}}\,\frac{e^{-[\Phi(m_R,\tau_\alpha)/kT]}}{\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,d\Delta}, \qquad p_\alpha^{+0} = k_l\sqrt{\frac{kT}{2\pi m}}\,\frac{e^{-[\Phi(m_R,\tau_\alpha)/kT]}}{\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,d\Delta} \tag{3.16$_2$}$$

$m$ is the mass of a lattice particle. The factors $k_l\sqrt{(kT/2\pi m)}$ and $k_c\sqrt{(kT/2\pi m)}$ represent the frequency with which the particles in the lateral potential wells and the central one are running against the barriers. The $k$'s are big for deep and narrow potential wells while they are small for flat and shallow ones. The exact values of the $k$'s remain in the theory as adjustable parameters, because our knowledge about the potential of the lattice particles is insufficient for their determination.

With the transition probabilities given, we easily write down the rate laws for $x_\alpha^\mp$ and $x_\alpha^0$ by means of the natural assumption that the number of particles leaving a certain phase is proportional to the number of particles in that phase. Thus we obtain

$$\begin{aligned}
\dot{x}_\alpha^- &= -x_\alpha^- p_\alpha^{-0} + x_\alpha^0 p_\alpha^{0-}, \\
\dot{x}_\alpha^0 &= +x_\alpha^- p_\alpha^{-0} - x_\alpha^0 p_\alpha^{0-} - x_\alpha^0 p_\alpha^{0+} + x_\alpha^+ p_\alpha^{+0}, \\
\dot{x}_\alpha^+ &= + x_\alpha^0 p_\alpha^{0+} - x_\alpha^+ p_\alpha^{+0}.
\end{aligned} \tag{3.17}$$

Of course, only two of these three equations are independent, because of the constraint (2.3).

The transition probabilities in eqns (3.16) are different for different orientations $\alpha$, because the shear force $\tau$ changes with $\alpha$, see eqn (3.8).

The rate laws eqns (3.4) and (3.17), for the deformation gradient and the phase factors, must now be supplemented by an equation for temperature.

3.3 *Temperature*

The rate equation that is needed for the temperature is based upon the balance of internal energy $U$ of the body, viz.

$$\frac{\mathrm{d}U}{\mathrm{d}t} + \oiint_{F(V)} q_i n_i \,\mathrm{d}f = \sigma_{ij}\dot{F}_{ik}F_{kj}^{-1}V. \tag{3.18}$$

$V$ and $F(V)$ are volume and surface of the body. We assume the heat flux to be proportional to the difference of the body temperature and the external temperature $T_E$, so that

$$\oiint q_i n_i \,\mathrm{d}f = W(T - T_E),$$

where $W$ is the heat-transfer number that depends on the properties on the body and of the surrounding medium, as well as on the size and shape of the surface.

Since the body consists of three phases, $U$ must be decomposed into three parts according to the equation

$$U = N\int_0^{\pi} g(\alpha, t)\left[x_\alpha^- \frac{\int_{-\infty}^{m_L} \Phi(\Delta, \tau_\alpha)\,\mathrm{e}^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,\mathrm{d}\Delta}{\int_{-\infty}^{m_L} \mathrm{e}^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,\mathrm{d}\Delta} + x_\alpha^0 \frac{\int_{m_L}^{m_R} \Phi(\Delta, \tau_\alpha)\,\mathrm{e}^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,\mathrm{d}\Delta}{\int_{m_L}^{m_R} \mathrm{e}^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,\mathrm{d}\Delta} + x_\alpha^+ \frac{\int_{m_R}^{\infty} \Phi(\Delta, \tau_\alpha)\,\mathrm{e}^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,\mathrm{d}\Delta}{\int_{m_R}^{\infty} \mathrm{e}^{-[\Phi(\Delta,\tau_\alpha)/kT]}\,\mathrm{d}\Delta}\right]\mathrm{d}\alpha + U_k(T). \tag{3.19}$$

The square bracket in the integrand represents the expectation value of the potential energy of a particle of orientation $\alpha$, and $N$ is the number of lattice particles in the body. $U_k(T)$ is the kinetic energy.

Upon differentiation of $U$ and insertion into eqn (3.18), we obtain the energy equation in the form

$$\begin{aligned}\left[N\int_0^{\pi} g(\alpha, t)R_\alpha\,\mathrm{d}\alpha + \frac{\mathrm{d}U}{\mathrm{d}t}\right]\dot{T} &= NfJ\int_0^{\pi} g(\alpha, t)\,(TS_\alpha - x_\alpha^- X_\alpha^- - x_\alpha^0 X_\alpha^0 - x^+ X_\alpha^+)\left(\frac{\partial\tau_\alpha}{\partial\alpha}\,\dot{\alpha} + \frac{\partial\tau_\alpha}{\partial\sigma_{ij}}\,\dot{\sigma}_{ij}\right)\mathrm{d}\alpha \\ &\quad - N\int_0^{\pi} g(\alpha, t)\,[(Y_\alpha^- - Y_\alpha^0)\dot{x}_\alpha^- + (Y_\alpha^+ - Y_\alpha^0)\dot{x}_\alpha^+]\,\mathrm{d}\alpha \\ &\quad - W(T - T_E) + \sigma_{ij}\dot{F}_{ik}F_{kj}^{-1}V,\end{aligned} \tag{3.20}$$

where, in addition to the definitions (3.10) and (3.12), the following definitions have been introduced:

$$Y_\alpha^- = \frac{\int_{-\infty}^{m_L} \Phi(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}{\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta},$$

$$Y_\alpha^0 = \frac{\int_{m_L}^{m_R} \Phi(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}{\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta},$$

$$Y_\alpha^+ = \frac{\int_{m_R}^{\infty} \Phi(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}{\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta}, \tag{3.21}$$

$$R_\alpha = \frac{1}{kT^2}\left\{ x_\alpha^- \frac{\left(\int_{-\infty}^{m_L} \Phi^2(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)\left(\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right) - \left(\int_{-\infty}^{m_L} \Phi(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)^2}{\left(\int_{-\infty}^{m_L} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)^2} \right.$$

$$+ x_\alpha^0 \frac{\left(\int_{m_L}^{m_R} \Phi^2(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)\left(\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right) - \left(\int_{m_L}^{m_R} \Phi(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)^2}{\left(\int_{m_L}^{m_R} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)^2}$$

$$\left. + x_\alpha^+ \frac{\left(\int_{m_R}^{\infty} \Phi^2(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)\left(\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right) - \left(\int_{m_R}^{\infty} \Phi(\Delta, \tau_\alpha)\, e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)^2}{\left(\int_{m_R}^{\infty} e^{-[\Phi(\Delta,\tau_\alpha)/kT]}\, d\Delta\right)^2} \right\}. \tag{3.22}$$

The factor of $\dot{T}$ in eqn (3.20) must be interpreted as the heat capacity of the body and it will henceforth be denoted by $C$.

Equation (3.20) is the desired rate law for $T$, which completes the set of eqns (3.4), (3.17) for the determination of $\mathbf{F}$, $x^\pm$, $x^0$ and $T$ as functions of time when $\sigma_{ij}(t)$ and $T_E(t)$ are known. Of course, $\dot{\alpha}$ in eqn (3.20) must be eliminated by (3.7), just as this has to be done in the eqns (3.4).

The most important term on the right-hand side of eqn (3.20) is the one with $Y_\alpha^- - Y_\alpha^0$ and $Y_\alpha^+ - Y_\alpha^0$, because that term represents the conversion of potential energy into kinetic energy as the phase changes occur; this contribution may be called the latent heat of the transformation.

### 3.4 *Summary of rate laws*

We summarize the rate laws for deformation gradient, phase fractions and temperature by writing the complete set of eqns (3.4), (3.17) and (3.26):

$$
\begin{array}{lclcccc}
\dot{F}_{11} & = & -I^{sc}(\dot{D})\,F_{11} & & (I^{cc}(\dot{D}) - I)\,F_{21} & \\
\dot{F}_{12} & = & & -I^{sc}(\dot{D})\,F_{12} & & (I^{cc}(\dot{D}) - I)\,F_{22} \\
\dot{F}_{21} & = & (-I^{ss}(\dot{D}) + I)\,F_{11} & & I^{sc}(\dot{D})\,F_{21} & \\
\dot{F}_{22} & = & & (-I^{ss}(\dot{D}) + I)\,F_{12} & & I^{sc}(\dot{D})\,F_{22} \\
\dot{x}_\alpha^- & = & -x_\alpha^-\,p_\alpha^{-0} & +x_\alpha^0\,p_\alpha^{0-} & & \\
\dot{x}_\alpha^0 & = & +x_\alpha^-\,p_\alpha^{-0} & -x_\alpha^0\,p_\alpha^{0-} & -x_\alpha^0\,p_\alpha^{0+} & +x_\alpha^+\,p_\alpha^{+0} \\
\dot{x}_\alpha^+ & = & & & +x_\alpha^0\,p_\alpha^{0+} & -x_\alpha^+\,p_\alpha^{+0}
\end{array}
$$

$$
\dot{T} = \frac{NfJ}{C}\int_0^\pi g(\alpha, t)\,[TS_\alpha - x_\alpha^- X_\alpha^- - x_\alpha^0 X_\alpha^0 - x_\alpha^+ X_\alpha^+]\left(\frac{\partial\tau_\alpha}{\partial\alpha}\,\dot{\alpha} + \frac{\partial\tau_\alpha}{\partial\sigma_{ij}}\,\dot{\sigma}_{ij}\right)\mathrm{d}\alpha
$$
$$
-\frac{N}{C}\int_0^\pi g(\alpha,t)[(Y_\alpha^- - Y_\alpha^0)\dot{x}_\alpha^- + (Y_\alpha^+ - Y_\alpha^0)\dot{x}_\alpha^+]\mathrm{d}\alpha - \frac{W}{C}(T - T_E) + \frac{V}{C}\sigma_{ij}\dot{F}_{ik}F_{kj}^{-1}. \tag{3.23}
$$

We have explained that the right-hand sides of these equations are known functions of the variables

$$
\mathbf{F},\dot{\mathbf{F}},T,\dot{T},x_\alpha^\pm,\dot{x}_\alpha^\pm,x_\alpha^0,\dot{x}_\alpha^0;\boldsymbol{\sigma},\dot{\boldsymbol{\sigma}},T_E, \tag{3.24}
$$

if only the potential $\Phi(\Delta, 0)$ and the initial distribution function $G(A)$ of orientations are given. In particular, the variables $\dot{\mathbf{F}}$, $\dot{T}$, $\dot{x}_\alpha^\pm$, $\dot{x}_\alpha^0$ occur linearly on the right-hand side of eqn (3.23).

If we remember the constraints (2.3) and (3.6), we conclude that the set of equations (3.27) constitutes a set of six integro-differential equations, which must be solved for given initial conditions and given functions $\boldsymbol{\sigma}(t)$ and $T_E(t)$.

For a numerical solution the set of six integro-differential equations is converted into a set of ordinary differential equations by discretizing the orientations $\alpha$. If there are $\nu$ orientations, we may formally combine the three independent components of $\mathbf{F}$, the 2 $\nu$ independent values among $x_\alpha^\pm$, $x_\alpha^0$ and the temperature in a vector $V_A(A = 1, 2, \ldots 2\nu + 4)$, and write eqn (3.27) in the form

$$
\dot{V}_A = \mathcal{D}_A(V_B;\boldsymbol{\sigma},\dot{\boldsymbol{\sigma}},T_E). \tag{3.25}
$$

We conclude that the development of the deformation, of the temperature and of phase fractions may be calculated as functions of time, if only the external stress $\boldsymbol{\sigma}$ and the external temperature $T_E$ are given as functions of time.

The actual calculation of $\mathbf{F}$ and $T$ requires a numerical evaluation of the eqns (3.23), and some results for particular choices of $\Phi(\Delta, 0)$ and $G(A)$ are reported in Section 5 below.

## 4. CONSTITUTIVE EQUATION

### 4.1. *Formulation*

Within the macroscopic theory of plasticity, a number of constitutive relations have been proposed for the calculation of the deformation in the elastic range and during creep and yielding. It is true that a memory alloy is not a plastic body in the ordinary sense of the word, but there are obvious similarities between the behavior of the two classes of bodies, and it is therefore conceivable that this paper might find some interest among researchers in plasticity.

For their benefit we reformulate the eqns (3.23) in order to cast that set of equations into a form that is easily comparable with the constitutive relations of plasticity.

Since the right-hand side of the rate laws $(3.23)_{5-7}$ for the phase fractions does not contain any rates, it is particularly easy to eliminate $\dot{x}_\alpha^\pm$ and $\dot{x}_\alpha^0$ from the eqns $(3.23)_{1-4}$ for $\dot{\mathbf{F}}$, and from eqn $(3.23)_8$ for $\dot{T}$. Also, since $\dot{\mathbf{F}}$ and $\dot{T}$ occur linearly in the eqns (3.23), we may solve for these derivatives and obtain equations of the general structure

$$\begin{aligned} \dot{\mathbf{F}} &= \mathcal{F}_1(\mathbf{F}, T, x_\alpha^-, x_\alpha^+, \boldsymbol{\sigma}) + \mathcal{F}_2(\mathbf{F}, T, x_\alpha^-, x_\alpha^+, \boldsymbol{\sigma})\dot{\boldsymbol{\sigma}}, \\ \dot{T} &= \mathcal{F}_3(\cdots) + \mathcal{F}_4(\cdots)\dot{\boldsymbol{\sigma}}. \end{aligned} \tag{4.1}$$

Equations like that are known in the theory of plasticity as constitutive equations of the flow type with internal variables. The internal variables are represented here by the phase fractions $x_\alpha^-$, $x_\alpha^+$

4.2. *Material frame indifference*

Equations of the form (4.1) are generally not relations between objective tensors, because neither $\dot{\mathbf{F}}$ nor $\dot{\boldsymbol{\sigma}}$ are objective tensors. However, in the present case $(4.1)_1$ is merely a drawn-out form of (3.1), whence it follows that $\dot{\boldsymbol{\sigma}}$ only occurs in the objective scalar combination $(\sigma_{ij} i_i^\alpha j_j^\alpha)^\cdot$, so that $\dot{\boldsymbol{\sigma}}$ presents no problem with respect to objectivity. Also, (3.1) may be written in the form

$$\dot{F}_{ij} - \int_0^\pi g(\alpha, t) \begin{pmatrix} 0 & -\dot{\alpha} \\ \dot{\alpha} & 0 \end{pmatrix}_{ik} F_{kj}\, d\alpha = \int_0^\pi g(\alpha, t) \frac{1}{h} \dot{D}_\alpha i_i^\alpha j_j^\alpha F_{kj}\, d\alpha, \tag{4.2}$$

so that for each $j$, both sides are objective vectors. Note that by (2.5) the integral over $g(\alpha, t)$ is equal to 1.

Material frame indifference is satisfied by this equation since the function $g(\alpha, t)$ is independent of frame.

## 5. SPECIAL CASES

5.1. *Scope*

The numerical effort in the solution of the system (3.23) is obviously considerable, if many orientations exist in the body; let alone, if there is a continuous distribution of orientations. The task of finding solutions will be much facilitated by the consideration of only few orientations.

Also, the calculations will be much simplified if we restrict the deformation by stipulating, for instance, that certain directions remain unchanged in the deformation. Such a stipulation may be physically reasonable for the appropriate loading. What remains is the task of determining the remaining components of $\mathbf{F}$ that are compatible with the constraint.

Another way of making things simpler by considering special cases concerns the external load. By eqn (3.8), the shear stress $\tau_\alpha$ is given by three external load functions, viz. $\sigma_{22}(t)$, $\sigma_{11}(t)$ and $\sigma_{12}(t)$. Obviously the situation can be made easier to handle by permitting only one of these functions to be present.

In the sequel we shall make use of all three of the above simplifications in order to demonstrate the potential of the model.

5.2. *Uniaxial deformation in a body with one orientation*

5.2.1. *Characterization.* We shall consider a body of whose initial configuration, Fig. 6, gives a schematic picture. Structure, load and deformation are special in three ways:

(i) The body contains only particles of a single orientation which we take to be 45 degree in the initial configuration. Thus we have

$$G(A) = \delta\left(\frac{\pi}{4} - A\right). \tag{5.1}$$

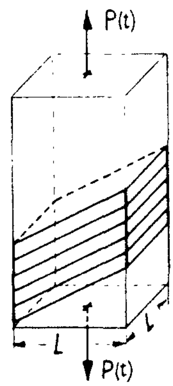


Fig. 6. Body with one shear direction in reference configuration.

(ii) The body is subject to a tensile or compressive load $P(t)$ in the 2-direction, see Fig. 6. Thus, by (3.8) $\tau_\alpha$ is given by

$$\tau_\alpha = \frac{\sigma_{22}}{2} \sin 2\alpha, \tag{5.2}$$

where $\sigma_{22}$ will be seen to be simply related to $P(t)$.

(iii) The vertical sides of the body remain vertical. This means that a unit vector **N** in the 2-direction is carried into the vector $\mathbf{n} = \mathbf{FN}$ which also points into the 2-direction. Therefore we must have $F_{12} = 0$.

The vertical load will produce a normal stress

$$\sigma_{22} = \frac{P(t)}{F_{11}L^2} \cdot \tag{5.4}$$

so that the shear stress $\tau_\alpha$ is given by

$$\tau_\alpha = \frac{P(t)}{2L^2} \frac{\sin 2\alpha}{F_{11}} \,. \tag{5.5}$$

5.2.2. *Rate laws for deformation.* In the present special case it will turn out that the rate laws for **F** can be integrated to give **F** in terms of $D_\alpha$, and there is only *one* function $D_\alpha(t)$, since there is only one orientation.

From eqn (2.11), we have with $A = \dfrac{\pi}{4}$ and $F_{12} = 0$,

$$\alpha(t) = \arctan \frac{F_{21} + F_{22}}{F_{11}} \quad \text{or} \quad \tan \alpha = \frac{F_{21} + F_{22}}{F_{11}}, \tag{5.6}$$

whence follows by differentiation

$$\dot{\alpha}(t) = \frac{1}{1 + \left(\dfrac{F_{21} + F_{22}}{F_{11}}\right)^2} \cdot \left(\frac{F_{21} + F_{22}}{F_{11}}\right)^{\cdot} \quad \text{or} \quad \frac{\dot{\alpha}(t)}{\cos^2 \alpha} = \left(\frac{F_{21} + F_{22}}{F_{11}}\right)^{\cdot}. \tag{5.7}$$

Since $g(\alpha, t)\, d\alpha = G(A)\, dA = \delta(A - (\pi/4))\, dA$ holds, the integrals $I$ of eqns (3.3) reduce to the form

$$I^{ss}(\dot{D}) = \frac{1}{h}\dot{D}_\alpha \sin^2\alpha, \qquad I^{sc}(\dot{D}) = \frac{1}{h}\dot{D}_\alpha \sin\alpha\cos\alpha,$$
$$I^{cc}(\dot{D}) = \frac{1}{h}\dot{D}_\alpha \cos^2\alpha, \qquad I = \dot{\alpha}, \tag{5.8}$$

where $\alpha$ and $\dot{\alpha}$ must be taken from eqns 5.6 and (5.7).

The eqns (5.8) may be used to simplify the rate laws (3.4) for the deformation gradient. They assume the forms

$$\dot{F}_{11} = -\frac{1}{h}\dot{D}_\alpha \sin\alpha\cos\alpha F_{11} + \left(\frac{1}{h}\dot{D}_\alpha\cos^2\alpha - \dot{\alpha}\right)F_{21} \tag{5.9$_1$}$$
$$\dot{F}_{12} = -\frac{1}{h}\dot{D}_\alpha \sin\alpha\cos\alpha F_{12} + \left(\frac{1}{h}\dot{D}_\alpha\cos^2\alpha - \dot{\alpha}\right)F_{22} \tag{5.9$_2$}$$
$$\dot{F}_{21} = \left(-\frac{1}{h}\dot{D}_\alpha \sin^2\alpha + \dot{\alpha}\right)F_{11} + \frac{1}{h}\dot{D}_\alpha\sin\alpha\cos\alpha F_{21} \tag{5.9$_3$}$$
$$\dot{F}_{22} = \left(-\frac{1}{h}\dot{D}_\alpha \sin^2\alpha + \dot{\alpha}\right)F_{12} + \frac{1}{h}\dot{D}_\alpha\sin\alpha\cos\alpha F_{22}. \tag{5.9$_4$}$$

$F_{12}$ is zero, so that $(5.9)_2$ implies $(1/h)D_\alpha \cos^2\alpha = \dot{\alpha}$, which, by use of eqn (5.7), may be written as

$$\frac{1}{h}\dot{D}_\alpha = \frac{\dot{\alpha}}{\cos^2\alpha} = \left(\frac{F_{21}+F_{22}}{F_{11}}\right)^{\cdot} \quad \text{or after integration, } \frac{1}{h}D_\alpha$$
$$= \tan\alpha - 1 = \frac{F_{21}+F_{22}}{F_{11}} - 1. \tag{5.10}$$

Therefore $(5.9)_1$ and $(5.9)_2$ reduce to

$$\dot{F}_{11} = -\frac{1}{h}\dot{D}_\alpha \sin\alpha\cos\alpha F_{11}$$
$$\dot{F}_{21} = \left(-\frac{1}{h}\dot{D}_\alpha\sin^2\alpha + \dot{\alpha}\right)F_{11} + \frac{1}{h}\dot{D}_\alpha\sin\alpha\cos\alpha\, F_{21}, \tag{5.11}$$

while $(5.9)_4$ merely implies

$$F_{22} = \frac{1}{F_{11}}, \tag{5.12}$$

which is equivalent to (3.6) for the present special case, where $F_{12} = 0$ holds.

By use of $(5.10)_1$ we may write $(5.11)_1$ in the form

$$\dot{F}_{11} = -\dot{\alpha}\tan\alpha F_{11}$$

or by integration (5.13)

$$F_{11} = \sqrt{2}\cos\alpha$$

or by $(5.6)_2$ and $(5.10)_2$

$$F_{11} = \frac{1}{\sqrt{\left[1 + \left(1 + \frac{1}{h}D_\alpha\right)^2\right]}}. \tag{5.14}$$

From eqns $(5.10)_2$, (5.12) and (5.14), the remaining two components of **F** can be derived, and we obtain

$$F_{21} = \sqrt{2}\,\frac{1 + \frac{1}{h}D_\alpha}{\sqrt{\left[1 + \left(1 + \frac{1}{h}D_\alpha\right)^2\right]}} - \frac{1}{\sqrt{2}}\sqrt{\left[1 + \left(1 + \frac{1}{h}D_\alpha\right)^2\right]}, \quad (5.15)$$

$$F_{22} = \frac{1}{\sqrt{2}}\sqrt{\left[1 + \left(1 + \frac{1}{h}D_\alpha\right)^2\right]}. \quad (5.16)$$

The remaining equation $(5.11)_2$ is identically satisfied by eqns (5.14)–(5.16) as can easily be checked.

By eqns (5.14)–(5.16) we have expressed all nonvanishing components of **F** in terms of $D_\alpha$, a quantity whose evolution is determined by the rate equation (3.9). Thus in the present case the set of four (or three) integro-differential equations (3.4) for **F** can be replaced by one ordinary differential equation for $D_\alpha$.

5.2.3. *Rate laws for phase fractions and temperature.* The rate laws (3.17) for the phase fractions remain unchanged. Of course there is only one orientation $\alpha$ now and, by eqns (5.4) and (5.12), we must replace $\tau$ in the transition probabilities (3.16) by

$$\tau_\alpha = \frac{1}{(\sqrt{2})L^2}P(t)\sqrt{(1 - \tfrac{1}{2}F_{11}^2)} = \frac{1}{(\sqrt{2})L^2}P(t)\sqrt{\left(1 - \frac{1}{1 + \left(1 + \frac{1}{h}D_\alpha\right)^2}\right)}. \quad (5.17)$$

The rate law (3.20) for temperature loses the integral because of eqn (5.1), and $\sigma_{ij}$ reduces to

$$\begin{pmatrix} 0 & 0 \\ 0 & \sigma_{22} \end{pmatrix},$$

so that we obtain by use of eqn (5.4)

$$C\dot{T} = -\frac{V}{L^2}\frac{1}{Nm}P(t)\frac{1}{F_{11}^2}\dot{F}_{11} - \frac{W}{Nm}(T - T_E(t)) + \frac{1}{m}[(Y_\alpha^- - Y_\alpha^0)\dot{x}_\alpha^-$$
$$+ (Y_\alpha^+ - Y_\alpha^0)\dot{x}_\alpha^+] + \frac{fh}{m}(TS_\alpha - x_\alpha^- X_\alpha^- - x_\alpha^0 X_\alpha^0 - x_\alpha^+ X_\alpha^+). \quad (5.18)$$

$c \equiv C/Nm$ is the specific heat. In this relation $\tau_\alpha$ must be replaced by eqn (5.17).

5.2.4. *Summary of Equations.* For easy reference we compile the equations that govern deformation, phase fractions and temperature in the present case.

$$\begin{aligned} \frac{1}{h}\dot{D}_\alpha &= K_\alpha\dot{\tau}_\alpha + S_\alpha\dot{T} + X_\alpha^-\dot{x}_\alpha^- + X_\alpha^0\dot{x}_\alpha^0 + X_\alpha^+\dot{x}_\alpha^+, \\ \dot{x}_\alpha^- &= -x_\alpha^- p_\alpha^{-0} + x_\alpha^0 p_\alpha^{0-} \\ \dot{x}_\alpha^0 &= x_\alpha^- p_\alpha^{-0} - x_\alpha^0 p_\alpha^{0-} - x_\alpha^0 p_\alpha^{0+} + x_\alpha^+ p_\alpha^{+0} \\ \dot{x}_\alpha^+ &= x_\alpha^0 p_\alpha^{0+} - x_\alpha^+ p_\alpha^{+0} \end{aligned} \quad (5.19)$$

$$c\dot{T} = \frac{1}{\sqrt{2}}\frac{V}{L^2}\frac{1}{Nm}P(t)\frac{\left(1+\frac{1}{h}D_\alpha\right)}{\sqrt{\left[1+\left(1+\frac{1}{h}D_\alpha\right)^2\right]}}\dot{D}_\alpha - \frac{W}{Nm}(T - T_E(t)) + \frac{1}{m}[(Y_\alpha^- - Y_\alpha^0)\dot{x}_\alpha^- + (Y_\alpha^+ - Y_\alpha^0)\dot{x}_\alpha^+] + \frac{fh}{m}[TS_\alpha - x_\alpha^- X_\alpha^- - x_\alpha^0 X_\alpha^0 - x_\alpha^+ X_\alpha^+]\dot{\tau}_\alpha.$$

Given $P(t)$ and $T_E(t)$, this is a system of equations for $D_\alpha$, $x_\alpha^\mp$, $x_\alpha^0$ and T. The coefficients $K_\alpha$, $S_\alpha$, $X_\alpha^\mp$ and $X_\alpha^0$ are defined in eqns (3.10)–(3.12). The transition probabilities are given by (3.16), and the potential differences $Y_\alpha^- - Y_\alpha^0$ and $Y_\alpha^+ - Y_\alpha^0$ may be read off from (3.21). All of these quantities depend on $\tau_\alpha$, and $\dot{\tau}_\alpha$ also appears explicitly in eqn (5.19). $\tau_\alpha$ and $\dot{\tau}_\alpha$ are related to $D_\alpha$ and $\dot{D}_\alpha$ by the equations

$$\tau_\alpha = \frac{1}{(\sqrt{2})L^2}P(t)\sqrt{\left(1 - \frac{1}{1+\left(1+\frac{1}{h}D_\alpha\right)^2}\right)}$$

and

$$\dot{\tau}_\alpha = \frac{1}{(\sqrt{2})L^2}\dot{P}(t)\sqrt{\left(1 - \frac{1}{1+\left(1+\frac{1}{h}D_\alpha\right)^2}\right)} + \frac{1}{(\sqrt{2})L^2}P(t) \times \frac{1+\frac{1}{h}D_\alpha}{\left[1+\left(1+\frac{1}{h}D_\alpha\right)^2\right]^2}\left\{\sqrt{\left(1 - \frac{1}{1+\left(1+\frac{1}{h}D_\alpha\right)^2}\right)}\right\}^{-1}\frac{1}{h}\dot{D}_\alpha, \tag{5.20}$$

but it is obviously impractical to use these relations in order to eliminate $\tau_\alpha$ and $\dot{\tau}_\alpha$ from eqn (5.19).

Once $D_\alpha$, $x_\alpha^\mp$, $x_\alpha^0$ and $T$ have been determined as functions of $t$ for particular choices of $P(t)$, and $T_E(t)$, the deformation gradient can be calculated from (5.14) through (5.16).

5.2.5. *Dimensionless variables.* The eqns (5.19) and (5.20) can be solved numerically, and for that purpose it is necessary to introduce dimensionless quantities. Generally speaking, the shear length $J$ and the barrier $B_0$ are used to make lengths and energies dimensionless. Forces, temperature and time are made dimensionless by combinations of the shear length $J$, the barrier $B_0$, the particle mass $m$ and the Boltzmann constant $k$. We define

$$\begin{aligned}
&\delta = \frac{\Delta}{J}, && \mu_{L,R} = \frac{m_{L,R}}{J}, && d_\alpha = \frac{D_\alpha}{J},\\
&\lambda^{\cdot} = \frac{X^{\cdot}}{J}, && \frac{1}{\gamma} = \frac{h}{J}, && \varphi = \frac{\Phi}{B_0},\\
&y_\alpha^{\cdot} = \frac{Y^{\cdot}}{B_0}, && \Theta = \frac{T}{B_0/k}, && p_\alpha = \frac{\tau_\alpha f}{B_0/J},\\
&p_E = \frac{1}{2}\cdot\frac{\frac{P(t)}{L^2}f}{B_0/J}, && k_\alpha = K_\alpha\frac{B_0}{fJ^2}, && s_\alpha = S_\alpha\frac{B_0}{kJ},\\
&\gamma_\alpha = R_\alpha\frac{1}{k}, && \hat{t} = t\sqrt{\left(\frac{B_0}{2\pi mJ^2}\right)}, && w = \frac{W}{C}\sqrt{\left(\frac{2\pi mJ^2}{B_0}\right)}.
\end{aligned} \tag{5.21}$$

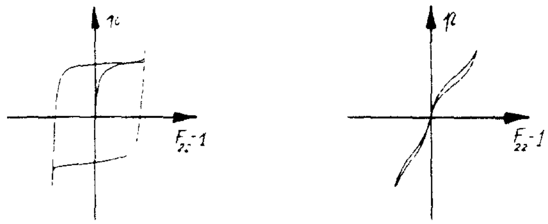

Fig. 7. Response to alternating tensile and compressive load at low and high temperatures.

$p_E$ is the dimensionless external force, while $p_\alpha$ is the nondimensional shear force on particles of orientation $\alpha$.

It will be assumed that the heat capacity $C$ is equal to $\mathcal{N}3k$, which conforms to the law of Dulong–Petit, when $\mathcal{N}$ is the total number of atoms. In the sequel we shall also use the characteristic quantity

$$\nu = \frac{N}{\mathcal{N}}, \tag{5.22}$$

which is the reciprocal of the number of atoms in a lattice particle.

5.2.6. *Results.* The Figs. 7 and 8 show the response of the model to an alternating tensile and compressive load $p_E(t)$ and a constant temperature $T_E$, which is low on the left hand side of the figures, 7, while on the right hand sides, it is high. The parameters of the model are given the values

$$\mu_L = \mu_R = 0,6;\ \lambda = 0,1;\ \gamma = 0,25;\ w = 1;\ \nu = 0,1;\ k_l = 10^4;\ k_c = 10^2, \tag{5.23}$$

where $\lambda$ is the ratio $\Phi(0)/B_0$, see Fig. 1. The maximum $|p_E^{max}|$ of the load is 0.5. The only difference between left and right in the two Figs. 7 and 8, is the external temperature, which has values

$$\Theta = \tfrac{1}{15} \quad \text{and} \quad \Theta_E = \tfrac{1}{6}, \tag{5.24}$$

respectively. This makes a lot of difference in the behavior of the model as is seen by a close study of Fig. 8.

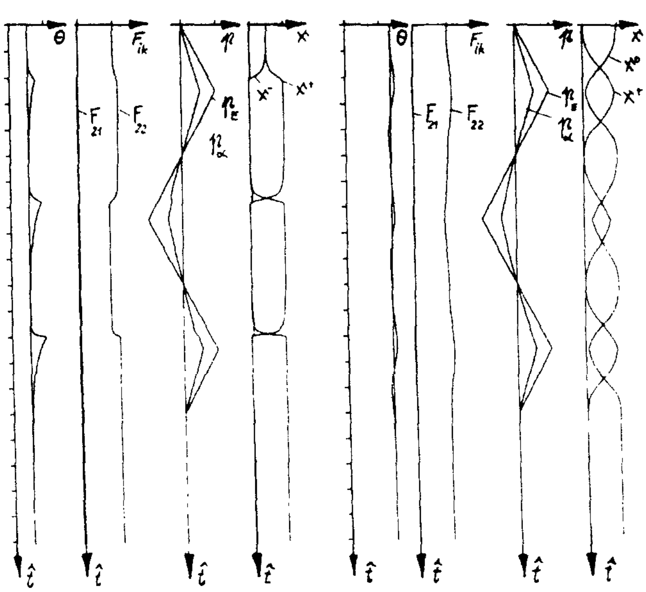

Fig. 8. Response to alternating tensile and compressive load at low and high temperatures.

The curves of Fig. 8 represent the phase factors, the angle $\alpha$, the shear stress $p_\alpha$, the deformation gradients $F_{22}$, $F_{12}$ and the temperature as function of time. Elimination of $\hat{t}$ between the functions $p_E(\hat{t})$ and $F_{22}(\hat{t})$ results in load-deformation diagrams, which exhibit most clearly the differences between the cases of low and high temperature. Those diagrams are shown in Fig. 7. At low temperature we see curves that are reminiscent of plastic behavior: In particular there is a fairly well-defined "yield load" and a hysteresis around the origin. [Unlike conventional plasticity, the yielding here is the consequence of a thermal activation, so that there is no prescribed yield limit (see [5]).]

At high temperature we see a typical pseudo-elastic behavior with separate hysteresis loops in the first and third quadrant.

It is most instructive to observe the transition between the phases. At low temperature we have only changes between the martensitic twins with austenite making a transient appearance as the changes occur. But at high temperature, all three phases are present at the appropriate loads, with austenite prevailing at small loads. This fact, of course, is the reason for the memory effect.

It is also interesting to point out that in the high-temperature case the temperature of the model oscillates around the external temperature. This is due to the fact that, upon yielding, the lattice particles convert potential energy into kinetic energy, i.e. heat by falling into the deeper potential well. On the other hand, in the recovery the particles convert kinetic energy into potential energy because the fastest ones are climbing out of the deep well; thus, in the recovery the body cools.

Both load-deformation curves in the Fig. 7 show a noticeable asymmetry between tension and compression. This can be traced back to the corresponding asymmetry of the shear stress $p_\alpha(\hat{t})$ is smaller since the load $p_E(\hat{t})$ is distributed over a bigger area.

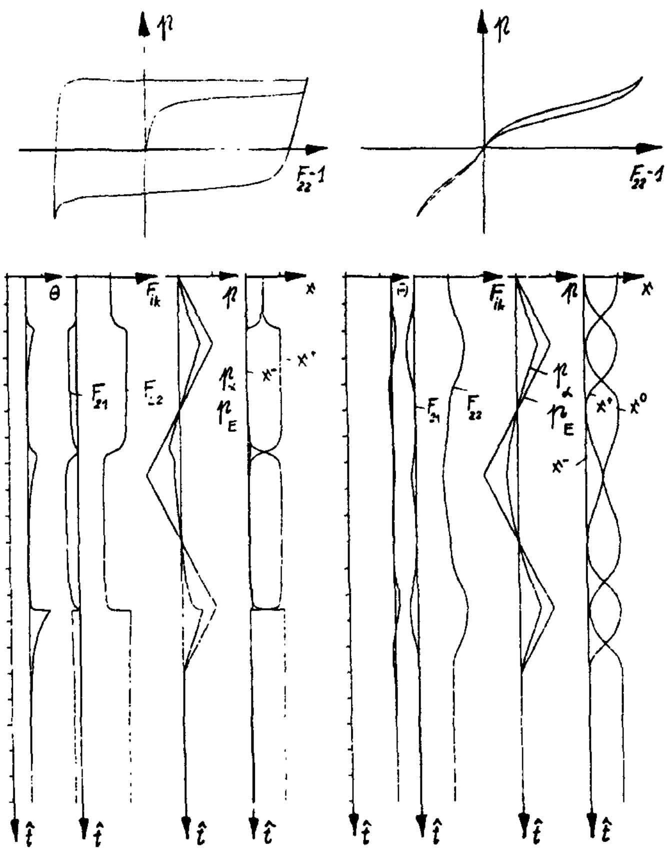

Fig. 9. Response to alternating tensile and compressive load at two temperatures. Asymmetry of stress–strain curves.

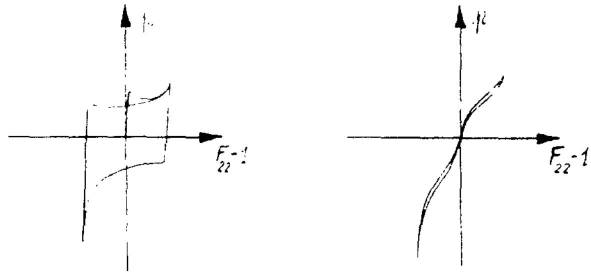

Fig. 10. Response to alternating positive and negative deformation at low and high temperatures.

The model has a considerable versatility which can be brought out by changing the parameters. An example is provided by Fig. 9, where the asymmetry in tension and compression is emphasized by choosing the ratio $\gamma = J/h$, three times as big as in eqn (5.23), leaving all other parameters unchanged. The temperatures are again given by (5.24).

So far the load has been prescribed and the resulting deformation has been calculated. One can also, of course, prescribe the deformation and calculate the corresponding load. The Figs. 10 and 11 give examples. The parameters are again given by eqn (5.23) and the temperatures by (5.24). The amplitude of the deformation is $|(F_{22} - 1)^{max}| = 0, 13$. There are two features of these curves that merit discussion.

The first one, noticeable at low temperature, is the softening which is exhibited after the body has reached the yield limit. This is due to the fact that many particles are ready to change from $M_-$ to $M_+$ once the yield load has been reached. Thus there could be a very rapid deformation at that load. But the rate of deformation is *prescribed* in this experiment, and it happens to be lower than the rate the body could achieve at the yield load. So, in order to accommodate the small rate of deformation, the load falls off.

The second feature to be discussed in the Figs. 10 and 11 is the marked asymmetry of the curves. We see that, while $p_\alpha(\hat{t})$ is fairly symmetric, $p_E(\hat{t})$ is not. In the compression, the lateral expansion of the body spreads the external force over a greater area so that more force is needed to make the lattice layers flip in compression than in tension.

Most of the features of the model discussed above can also be observed in experiments with memory alloys. In particular the general form of the load deformation

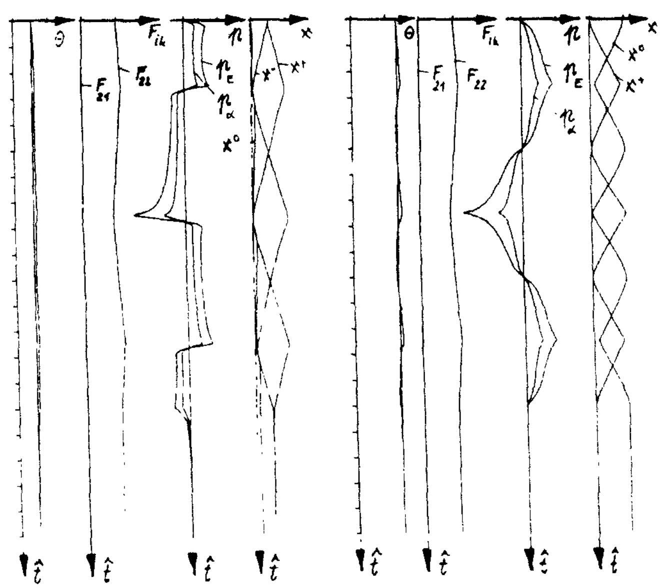

Fig. 11. Response to alternating positive and negative deformation at low and high temperatures.

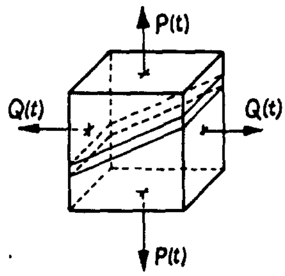


Fig. 12. Body under biaxial loading.

curves of the Fig. 7 strongly resemble observed curves. However, not all is quite well. Indeed, it is appropriate also to point here to a shortcoming of the model: At high temperature the width of the hysteresis loops depend on the frequency of the load function. At a very small frequency the hysteresis vanishes and the model becomes truly elastic. This is a feature of the model that does not reflect the behavior of a memory alloy. That situation calls for an improvement of the model which will be described in a future paper.

5.3. *Biaxial tension and compression*

5.3.1. *Differences between biaxial and uniaxial loads.* We continue to consider only one orientation with the initial value $\pi/4$ and the constraint $F_{12} = 0$. However, we shall allow normal forces to act on the lateral sides of the body so that $\sigma_{22}$ and $\sigma_{11}$ are both unequal to zero. In that case we have by eqn (3.8)

$$\tau_\alpha = \frac{\sigma_{22} - \sigma_{11}}{2} \sin 2\alpha,$$
$$\tau_2 = \frac{1}{2L^2}\left(\frac{P(t)}{F_{11}} - Q(t)F_{11}\right) \sin 2\alpha. \tag{5.25}$$

$P(t)$ and $Q(t)$ are the vertical and horizontal loads, respectively, see Fig. 12.

The formulae governing this case are quite similar to those of the uniaxial load treated in Section 5.2. In particular $\alpha$ is still given by eqn (5.6), and therefore $\tau_\alpha$ by eqn (5.25) may be written as

$$\tau_\alpha = \frac{1}{(\sqrt{2})L^2}[P(t) - Q(t)F_{11}]\sqrt{\left(1 - \frac{F_{11}^2}{2}\right)}$$
$$= \frac{1}{(\sqrt{2})L^2}\left(P(t) - Q(t)\frac{2}{1 + (1 + \frac{1}{h}D_\alpha)^2}\right)\sqrt{\left(1 - \frac{1}{1 + \left(1 + \frac{1}{h}D_\alpha\right)^2}\right)}. \tag{5.26}$$

This differs from eqn (5.17) by the term with $Q(t)$. Apart from that difference, there is only one more between the uniaxial and biaxial case and that concerns the power term in eqn (5.19). This term is now given by the expression

$$-\frac{V}{L^2}\cdot\frac{1}{Nm}\cdot(P(t) - Q(t)F_{11}^2)\cdot\frac{\dot{F}_{11}}{F_{11}^2} = \frac{1}{\sqrt{2}}\cdot\frac{V}{L^2}\cdot\frac{1}{Nm}$$
$$\cdot\left(P(t) - Q(t)\frac{2}{1 + \left(1 + \frac{1}{h}D_\alpha\right)^2}\right)\frac{1 + \frac{1}{h}D_\alpha}{\sqrt{\left[1 + \left(1 + \frac{1}{h}D_\alpha\right)^2\right]}}\dot{D}_\alpha. \tag{5.27}$$

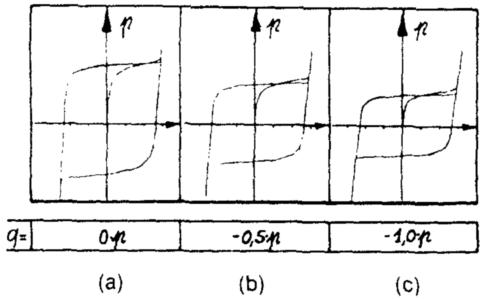


Fig. 13. Lowering of the yield limit by lateral compression.

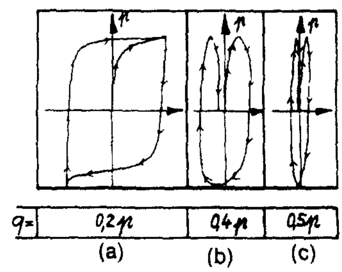


Fig. 14. Increase of the yield limit by lateral tension.

Thus the biaxial case is only a little more complex than the uniaxial case, and the greater complexity is quite unimportant for the numerical evaluation.

5.3.2. *Results.* Figure 13 shows an instructive example for the effect of a biaxial load upon a body. It gives three examples in which

$$p_E(t) = \frac{1}{2} \cdot \frac{\frac{P(t)}{L^2} f}{B_0/J}$$

and

$$q_E(t) = \frac{1}{2} \cdot \frac{\frac{Q(t)}{L^2} f}{B_0/J}$$

are both zig-zag curves in tension and compression but in opposite phase, i.e. when $p_E$ is a tensile load, $q_E$ is compressive and vice versa. In all three figures $| p_E^{\max} |$ equals 0.5, while $| q_E^{\max} |$ is chosen as 0, $-0.5p_E$ and $-p_E$, respectively. The load-deformation curve of Fig. 13(a) is identical to that of Fig. 7, since it represents a uniaxial loading and all parameters are chosen the same. The presence of $q_E$ in the Figs. 13(b) and 13(c) decreases the yield load, since the lateral expansion that results from $q_E(t)$ helps the load $p_E(t)$ to extend the body in the 2-direction.

This influence of the biaxial loading upon the yield load is confirmed by Fig. 14. Here the yield load is increased, because $p_E(t)$ and $q_E(t)$ are in phase. This fact leads to the strange looking curves of Figs. 14(b) and 14(c). Here the yield load has surpassed the amplitude of $p_E$, so that only a little creep can occur before the external load falls off again. The diagrams of Fig. 14 also show that there is less and less deformation when the amplitude of $q_E$ approaches that of $p_E$. For equal amplitudes there would be no deformation at all, since the model can only undergo isochoric motion.

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