Theory of Multilayer SMA Actuators

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Two types of multilayer actuators based on a shape memory alloy (SMA) film as an active component are explored theoretically. One of them uses the bending of an actuator due to the movement of an austenite/martensite interface of a SMA film parallel to a film plane. Another type of actuation uses the combination of passive layers with different coefficients of thermal expansion for engineering curvature. It is shown that in both cases the actuating deformation of the multilayer actuators can be optimized by the combination of the layers with different elastic properties, misfits and thickness.

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1. Introduction

Advanced technology stimulates an interest in phase transformations and the microstructure evolution in thin films. Transformable films allow one to obtain large displacements accompanying phase transformations with a relatively small transformational self-strain. This makes possible to use transformable films as efficient sensors and actuators. In contrast with many works which consider bending of bi-layer films consisting of a transforming (active) film on a passive substrate (e.g. see recent paper1–4) we consider films or plates containing more than two active and passive layers.

After the analysis of the mechanics of a film bending due to non-uniform transverse distribution of self-strain the two design principles of the actuator are considered:

(1) bending as a result of movement of the front of martensitic transformation parallel to a SMA film plane;
(2) manipulating a bend curvature by using a combination of passive layers with different coefficients of thermal expansion.

These examples demonstrate that by using multilayer films it is possible to expand functions and to enhance the performance of SMA actuators.

SMA actuators are usually used as cantilevers or membranes. In the first case the curvature and deflection are determined mainly by the evolution of stain and internal stress in an actuator. The effect of external forces at the fixed end of cantilever can be neglected when the actuator performance due to changing temperature is considered. In the case of membrane the average displacement curvature is a result of the equilibrium between the internal stresses and external forces at the edge of membrane. In this paper the effect of boundary conditions is not considered and therefore, the results can be applied to the cantilever although some comments on the membrane are made.

2. Internal Stress, Curvature and Elastic Energy of a Multilayer Film

Consider a multilayer plate with a thickness 2L, much smaller than the in-plane dimensions (L′) (Fig. 1). Then, the elastic problem becomes one dimensional. The plate consists of infinitely thin misfitted layers, so a misfit self-strain is a continuum function of the coordinate of the layer, z, along the axes normal to the plate, n. The local internal stress is

\[ \sigma(z) = C(\varepsilon(z) - \varepsilon^0(z)) \] (1)

where \( \varepsilon(z) \) is a total strain, \( \varepsilon^0(z) \) is the self-strain of the layer with coordinate \( z \), and \( C \) is an elastic modulus tensor. The total strains should be compatible, i.e. they should satisfy the following equation of compatibility:

\[ \nabla \times \varepsilon(z) \times \nabla = 0, \quad \nabla \equiv \frac{d}{dz} \] (2)

The solution of eq. (2) is as follows

\[ \varepsilon(z) = \frac{1}{2} (\delta(z) \cdot n + \varepsilon(z) \cdot \hat{n}) + \hat{k}z \] (3)
where \( \hat{\varepsilon} \) and \( \hat{\kappa} \) are the integration constants (\( \hat{\kappa} \) is a curvature tensor). The displacement \( \vec{\delta}(z) \) follows from the equation of mechanical equilibrium \( \vec{\delta} = 0 \):

\[
\vec{\delta}(z) = (\vec{n}C\vec{n})^{-1}\vec{n}C[\hat{\varepsilon}_0(z) - \hat{\varepsilon} - \hat{\kappa}z]
\]

The internal stress (eq. 1) is as follows:

\[
\hat{\sigma}(z) = G(\hat{\varepsilon} + \hat{\kappa}z - \hat{\varepsilon}_0(z))
\]

(5)

where \( G \) is a planar elastic modulus given by:

\[
G = C - \varepsilon^0 G\vec{n}(\vec{n}C\vec{n})^{-1}\vec{n}C
\]

(6)

\[
G_{ijkl} = C_{ijkl} - C_{ijkl}n^i n^j \varepsilon^0 \gamma^k \gamma^l
\]

(7)

The constants \( \hat{\varepsilon} \) and \( \hat{\kappa} \) are determined by the requirement that the average internal stress and the average momentum of internal stress should be equal to zero:

\[
\int_{-L}^{L} \sigma(z)dz = 0, \quad \int_{-L}^{L} z\sigma(z)dz = 0
\]

(8)

Then,

\[
\hat{\varepsilon} = \frac{1}{2L} \int_{-L}^{L} \hat{\varepsilon}_0(z)dz, \quad \hat{\kappa} = \frac{3}{2L^2} \int_{-L}^{L} z\hat{\varepsilon}_0(z)dz.
\]

(9)

The elastic energy is

\[
E = \frac{1}{2} \int_{-L}^{L} \hat{\sigma}(z)\hat{\varepsilon}_0(z)dz
\]

\[
= \frac{1}{2} \int_{-L}^{L} (\hat{\varepsilon} + \hat{\kappa}z - \hat{\varepsilon}_0(z))G(\hat{\varepsilon} + \hat{\kappa}z - \hat{\varepsilon}_0(z))dz
\]

\[
= \frac{1}{2} \int_{-L}^{L} \hat{\sigma}(z)\hat{\varepsilon}_0(z)dz
\]

\[
= \frac{1}{2} \int_{-L}^{L} (\hat{\varepsilon}_0(z)G(\hat{\varepsilon} + \hat{\kappa}z - \hat{\varepsilon}_0(z))dz
\]

(10)

The first line of eq. (10) transforms to the second one by using eq. (8). For example if \( \hat{\varepsilon}_0(z) \) is a step-like function

\[
\hat{\varepsilon}_0(z) = \begin{cases} 0 & \text{if } -L < z < L - h \ \\ \hat{\varepsilon}_0 & \text{if } L - h < z < L \end{cases}
\]

(11)

we obtain

\[
\hat{\varepsilon} = \alpha\hat{\varepsilon}_0, \quad \hat{\kappa} = 3\hat{\varepsilon}_0(1 - \alpha)\frac{L}{L'}
\]

(12)

\[
\sigma_1(z) = G\hat{\varepsilon}_0 \left[ \alpha + 3(1 - \alpha) \frac{z}{L} \right], \quad -L < z < L - h
\]

\[
\sigma_2(z) = G\hat{\varepsilon}_0 \left[ \alpha - 1 + 3(1 - \alpha) \frac{L}{L'} \right], \quad L - h < z < L
\]

(13)

where

\[
\alpha = \frac{h}{2L}, \quad 1 - \alpha = \frac{2L - h}{2L}
\]

The elastic energy in the plate according to eq. (10) is

\[
E(\alpha) = \frac{1}{2} \int_{-L-h}^{L-h} \hat{\sigma}_2(z)dz
\]

and with eq. (13) the average density of the energy in the plate is

\[
e(\alpha) = \frac{E(\alpha)}{2L} = \frac{1}{2} \hat{\varepsilon}_0 G\hat{\varepsilon}_0[(1 - \alpha)(1 - 3\alpha) - (1 - \alpha)]
\]

\[
= \frac{1}{2} \hat{\varepsilon}_0[(1 - \alpha)(1 - 3\alpha)]
\]

(15)

The elastic energy for bending film is shown in Fig. 2. The case when the elastic moduli of the layers are identical is considered here for simplicity, although the result can be generalized for the different moduli also.

3. Martensitic Transformation in a Bending Film

To explore a martensitic transformation in a free standing film we consider a model phase transformation from phase 1 to phase 2 accompanied by a self-strain, \( \varepsilon_0^{01} \). Coexisting phases are coherent, i.e. the total strains in a two-phase state are compatible, including an interface between phases. It means that there is no plastic deformation or fracture during the transformation.

It is assumed that the mismatch between the phases is minimal along the interface parallel to a film plane. Then a preferable configuration of a two-phase state is a layer structure with interfaces parallel to a film plane. This configuration corresponds to a minimum of elastic energy of internal stresses, if elastic moduli of the phases are identical. The trend to minimize the surface energy of interfaces dictates the heterophase microstructures with a minimal number of phase layers. This is a two-layer microstructure shown in Fig. 1.

The bi-layer film bends during the phase transformation. The elastic energy per unit of the film volume is determined by eq. (15); the energy

\[
e_0 = \frac{1}{2} G_{ijkl} e_0^{01} e_0^{01}
\]

(16)

is a characteristic energy of mismatch depending on a self-strain \( e_0^{01} \) and on the orientation of interface. If \( e_0^{01} = e_0 \delta_{ik} \) is a pure dilatation or a dilatation in a film plane, the elastic energy for isotropic case is equal to

\[
e_0 = E e_0^{01}/(1 - v)
\]

(17)

where \( E \) is the Young’s modulus, \( v \) is the Poisson ratio. This energy corresponds to a polycrystalline film without texture, since the average self-strain is equal to a volume effect of a
The free energy density of a two-phase film depends only on one variable parameter: a fraction of the phase \( 2, \alpha \):

\[
F(\alpha) = (1 - \alpha) f_1 + \alpha f_2 + e(\alpha) + \frac{\gamma}{2L} \\
= f_1 + \Delta f \alpha + e(\alpha) + \frac{\gamma}{2L}
\]

where \( \Delta f = f_2 - f_1 \) is a free energy difference, \( \gamma \) is a specific surface energy of the interface. The equation of phase equilibrium \( dF/d\alpha = 0 \) leads to the equations which determine an equilibrium phase fraction:

\[
\Delta f + \frac{de(\alpha)}{d\alpha} = 0
\]

or

\[
\Delta f + \frac{1}{2}(\hat{\sigma}_1 + \hat{\sigma}_2)\hat{\varepsilon}_0 = 0
\]

where \( \hat{\sigma}_1 \) and \( \hat{\sigma}_2 \) are stresses on the both sides of the interfaces at \( z = L - h \) (eq. (13)). The equilibrium two-phase state is stable if \( d^2F/d\alpha^2 = d^2e/d\alpha^2 \geq 0 \) and is unstable otherwise.

It is convenient to introduce here dimensionless parameters:

\[
\phi = \frac{\Delta f}{e_0}; \quad u(\alpha) = \frac{e(\alpha)}{e_0}
\]

Since \( \Delta f = q(1 - T/T_0) \) (\( q \) is a latent heat), \( \phi \) can be considered as "temperature" counting from the temperature of the phase equilibrium \( T_0 \). The equilibrium eq. (19) reduces to

\[
\phi + u'(\alpha) = 0
\]

which is a minimizer of the free energy

\[
\Phi(\alpha) = \phi \alpha + u(\alpha)
\]

(the free energy of phase 1 is taken as a reference state). Hereafter the change of interface energy is neglected because the thickness of the film is supposed to be much larger than \( \gamma/e_0 \), i.e. the elastic energy dominates.

There are equilibrium two-phase states for a bending film if \( 1/3 < \alpha < 2/3 \), when

\[
u''(\alpha) = -8 + 36\alpha(1 - \alpha) \geq 0
\]

These states are metastable because their energies are higher than the energy of one of the single-phase states (Fig. 3). These metastable states cannot be reached at cooling or heating of a single-phase state. The necessary condition of the onset of the coherent transformation is

\[\Delta f + e_0 \leq 0\]

\[\phi < -u'(0) = -1 \text{ at } 1 - 2 \text{ transformation}\]

\[\phi > u'(1) = +1 \text{ at } 2 - 1 \text{ transformation}\]

The solution of an equilibrium equation

\[
\phi + (1 - 2\alpha)(1 - 6\alpha(1 - \alpha)) = 0
\]

is presented in Fig. 3 as \( \phi(\alpha) \) curve. The sections \( 0 < \alpha < 1/3 \) and \( 2/3 < \alpha < 1 \) correspond to unstable barrier states. The section \( 1/3 < \alpha < 2/3 \) corresponds to metastable states. There are cusp minima of \( \Phi(\alpha): \alpha = 0 \) at \( \phi \geq -1 \) and \( \alpha = 1 \) at \( \phi \leq +1 \). Therefore, the system remains in a single phase state until the critical undercooling or overheating is obtained and an initial single-phase state becomes unstable. Then, the system jumps in a new single-phase state. Thus, a bending film transforms with the same hysteresis as an unbent film does\(^7\) (Fig. 3(a)).

However, the film can be trapped in the metastable state between \( \alpha = 1/3 \) and \( \alpha = 2/3 \) if the bending is restricted or not all thickness of the film is accessible for transformation. Then, the two-phase state can reversibly change during heating-cooling provided the phase fraction \( \alpha \) remains within the \( 1/3 < \alpha < 2/3 \) interval (Fig. 3(b)). Correspondingly to the phase evolution, the film should bend reversibly demonstrating a two-way shape memory effect. For example, combining transforming film with a thin substrate it is possible to maintain the reversible transformation after a film has been heat from the low temperature phase to the high temperature phase and then it thermocycling in restricted interval of temperature (Fig. 4). If the elastic properties of a substrate are close to those of the film and there is no misfit between the substrate and the film in a high temperature phase, the substrate should have a thickness equal to a half of the film thickness. To maintain two-way bending the top non-transforming layer of an austenite can be substitute by a top passive layer.

The model considered above presents simplified picture of martensite-austenite transformation in a bending film. It is assumed that the interface between austenite and martensite layers is sharp, i.e. a transient two-phase zone is thin. The self-strain, \( \varepsilon_0 \), as well as free energy of martensite, \( f_1 \), de-
The common concept of shape-memory alloy actuator is based on the relaxation of thermal stress in SMA film/substrate bimorph. The stress relaxation in a bimorph is determined by the evolution of austenite-martensite microstructure during the transformation. The main parameters of the microstructure are the fractions of the phases and domain composition of a polydomain martensite. To illustrate how the evolution of these parameters affects bimorph actuation we consider a cubic-tetragonal transformation in the film deposited on the thick substrate $^{9,10}$.

The three domains of a tetragonal martensite correspond to the following self-strains (Fig. 5(a)):

$$
\hat{\varepsilon}_0^1 = \varepsilon_0 \begin{pmatrix} 2 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} 
$$

$$
\hat{\varepsilon}_0^2 = \varepsilon_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix} 
$$

$$
\hat{\varepsilon}_0^3 = \varepsilon_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} 
$$

The free energy of the two-phase microstructure in the film is as follows:

$$
f(\beta, \alpha) = f_1^0 + \alpha \Delta f + \frac{E}{1 - \nu} (\varepsilon - \alpha \varepsilon_0(\beta))^2 
$$

where $\alpha$ is a fraction of the martensite and $\beta$ is a domain fraction. The last term is a constraint energy expressed through the isotropic biaxial stress, $\sigma = \frac{E}{1 - \nu} (\varepsilon - \alpha \varepsilon_0(\beta))$, with in-plane components of misfit, $\varepsilon$, and an average self-strain $\alpha \varepsilon_0(\beta)$ (Fig. 5(b)). Due to isotropy of the misfit the self-strain corresponding to an equilibrium has to be isotropic also and the microstructure should contain equal fractions of domain (1) and (2) as follows

$$
\varepsilon_0(\beta) = (1 - \beta) \frac{1}{2} (\hat{\varepsilon}_0^1 + \hat{\varepsilon}_0^2) + \beta \hat{\varepsilon}_0^3 
$$

with in-plane components $\varepsilon_{11}(\beta) = \varepsilon_{22}(\beta) = \varepsilon_0(\beta) = \frac{1}{2} (1 - 3\beta) \varepsilon_0$ where $\beta$ is a fraction of domain 3. In the austenite-martensite microstructure the domains are assembled into polytwins martensite plates compatible to the austenite. $^9$ The density of the local free energy of martensite, $f_2$, in the thermodynamic driving force $\Delta f = f_2 - f_1$, should include energy of interfaces and internal stresses between martensite plates forming local martensitic microstructure.

Fig. 4 The reversible transformation in the film on the substrate after the martensite state in the film is reached under cooling.

Fig. 5 Martensitic transformation in constrained film. (a) Domains of cubic-tetragonal transformation. (b) Strains in the bimorph.
The equilibrium fraction, \( f \) obtained for maximum of (1 through the change of domain fraction (twinning). The stress is a result of superplastic deformation of martensite which shifts the phase equilibrium from the equation of equilibrium phase

\[
\beta f \sigma = \Delta f (T \alpha - T \beta) \leq \varepsilon \mathrm{d}
\]

The main features of evolution of stress and microstructure in a transforming film during cooling of a bimorph actuator considered above is general for all types of martensitic transformations in single crystalline or polycrystalline SMA films. Upon cooling and increasing thermal stress, the transformation starts as a stress-induced one with maximal strain effect to obtain the maximal stress relaxation. Decreasing stress controls the degree of transformation. If the thermal stress is large, the stress-induced transformation ends at temperature higher than \( T_0 \). The stress remains positive.

If the thermal stress is small, the transformation does not end before temperature reaches \( T_0 \) and the stress induce transformation becomes the stress-assistant one when chemical driving force (\( \Delta f \)) becomes negative. In this case the degree of transformation as well as the martensite microstructure are determined rather by temperature than by stress. This martensite microstructure is superplastic, i.e. it can easily change under stress, and maintains the minimal level of stress in the bimorph upon further cooling. Particularly, the stress in the bimorph can be equal to zero. This “invar effect” due to the superplasticity of martensite has been observed recently.11)

5. Inverse Curvature of SMA Actuators

The martensitic transformation in an active film of bimorph actuator consisting of a thin transforming layer and a thick substrate leads to relaxation of thermal stress due to layer misfit. Therefore, the stress in the active film cannot change its sign during the transformation and the curvature of the bimorph does not change its sign as well (Fig. 8(a)). However, it is possible to engineer an actuator with a curvature and a deflection changing its sign due to a transformation if a third layer with specially determined parameters is interleaved.

If the thickness of this layer, \( h_i \), as well as thickness of the SMA film, \( h_f \), are small in comparison to the thickness of the substrate, \( H \), the stresses in both layers are determined by their misfit with the substrate layer, i.e. \( \sigma_i = \frac{E_i}{E^*} \varepsilon_i = \frac{E_i}{E^*} \Delta \theta (T - T_0) \) where \( \varepsilon_i \) is the misfit between intermediate layer and substrate, \( \Delta \theta \) is the difference of the thermal expansions of the intermediate and substrate layers, \( E_i \) is the Young’s modulus of the intermediate layer. If the sign of \( \Delta \theta \) is opposite to the sign of \( \Delta \theta \), the average biaxial stress in this
using the bi-layer (Fig. 7). This result follows directly from stress in the bi-layer and a configuration of the membrane containing SMA film and an intermediate layer.

\[ \sigma = \frac{1}{h_i + h_f} (\sigma_i h_i + \sigma_f h_f) \]  

(30)
can change its sign during transformation as it is shown in Fig. 7(c). The curvature of the active film/intermediate layer/substrate trimorph if \( h_f \ll H \) and \( h_i \ll H \) is approximately equal to \( \kappa = \frac{h_i + h_f}{H^2} \langle \sigma_i h_i + \sigma_f h_f \rangle (1 - v_i)^{12} \). The curvature changes its sign according to the change of sign of the average stress in the bi-layer (Fig. 7). This result follows directly from the equality of in-plane dimensions of the both thin layers and the substrate.

The curvature of trimorph in general case is determined by eq. (9). Particularly, the curvature is equal to zero if

\[ \varepsilon_f \delta_1 (1 - 2\delta_2 - \delta_1) + \varepsilon_f \delta_2 (1 - \delta_2) = 0 \]  

(31)
where \( \varepsilon_f \) is a difference of self-strains of an active layer and a substrate, \( \delta_1 = h_i / H \), \( \delta_2 = h_f / H \). The elastic moduli of the active layer and substrate are assumed to be the same.

Since the average stress in the bi-layer can change from extension to compression as a result of martensitic transformation in the SMA film, it is possible to induce a large deflection using the bi-layer \( h_f + h_i \) as a membrane (Fig. 7(c)). Because the thermal expansion of an intermediate layer is less than the one of the substrate, the membrane containing only an intermediate layer would be bent at cooling as shown in Fig. 8(a). The deflection of the spherical membrane can be calculated approximately (Fig. 8(b)) taking into account that the radius of membrane, \( R \), changes on \( \Delta \theta \) (32).

\[ \frac{d}{R} = \sqrt{2(T - T_R)} \Delta \theta \]  

(32)
The SMA layer with the thermal expansion coefficient larger than the thermal expansion coefficient of the substrate is in the extension state and arrests the bending of the membrane. Relaxation of stresses in the SMA film due to the transformation triggers bending of the membrane. In particular, the formation of superplastic martensite in the SMA film, leads to the bending of the membrane as if the membrane contains only an intermediate layer.

As an example consider the bending of a composite membrane NiTi/SiO\(_2\) on Si substrate. As it is observed in \(^{13}\) this membrane has zero curvature before transformation in the NiTi film and it is bent after the transformation. The thickness of the NiTi film, SiO\(_2\) layer and Si-substrate are as follows: \( h_f = 3 \mu m, h_i = 1 \mu m, H = 350 \mu m \), respectively; i.e. \( h_i \ll H, h_f \ll H \) and the relative thickness of the NiTi film, \( h_f / (h_i + h_f) = 0.75 \). The average stress in the membrane can be calculated using eq. (30) and the experimental data on stress-temperature dependence of NiTi film. Since the thickness of NiTi film is relatively large, the change of sign of the average stress in the membrane is possible only if the stress in the NiTi film is almost relaxes. Thus, the average stress in the membrane becomes negative and the bending the membrane occurs at temperature, \( T^* \), lower than \( M_s \). The analysis of stress and microstructure evolution in the bending membrane is a complex problem. However, the magnitude of the deflection of the membrane can be estimated according to eq. (32). Using the coefficients of thermal expansion for SiO\(_2\) and Si as \( 0.5 \times 10^{-6} \) and \( 3 \times 10^{-6} \), respectively, and \( T_R = 600 \text{ K}, \text{ the deflection at } T = 320 \text{ K is } 3.7 \times 10^{-4} \). The deflection of the membrane measured experimentally \(^{13}\) \( (d/R) \) at \( T = 320 \text{ K is } 4.2 \times 10^{-4} \). Thus, this estimation of the magnitude of deflection of the membrane agrees well with experimentally observed deflection.
6. Conclusions

The problems considered in this paper are the parts of a more general problem of transformation in the graded plates resulting in its bending. The non-uniform transformation throughout thickness of the active layer can be induced by the temperature gradient, external stresses or it can be result of non-uniform structure of the layer, e.g., non-uniform composition or defect distribution. The theory introduced in this paper based on the analysis of equilibrium states does not pretend to quantitatively describe the evolution of microstructure and the deformation in the multilayer films. However, this thermodynamic theory clearly demonstrates the opportunities for design of multilayer actuators with different functional properties.

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REFERENCES

5) The following notations are used in the paper: vectors: normal \( \vec{n} \), displacement \( \vec{s} \); 2nd rank tensors: strain \( \hat{\varepsilon} \), stress \( \hat{\sigma} \) with components: \( \varepsilon_{ij} \), \( \sigma_{ij} \) \((i, j = 1, 2, 3)\); 4-th rank tensors: elastic modulus \( C \), compliance \( S \), planar elastic modulus \( G \); \( \hat{\sigma} \Rightarrow \sigma_{ij}, \hat{\varepsilon} \Rightarrow \varepsilon_{ij}, C \Rightarrow C_{ijkl}, \hat{\varepsilon}C \Rightarrow \varepsilon_{ij}C_{ijkl}\varepsilon_{kl}, \hat{\sigma} \Rightarrow \sigma_{ij}, \hat{\varepsilon} \Rightarrow \varepsilon_{ij}, \hat{\varepsilon}C \Rightarrow \varepsilon_{ij}C_{ijkl}\varepsilon_{kl} \).