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Actuation based on phase transformations in microlayered architectures

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Abstract. The influence of phase transformations on the actuation capacity of microlayered architectures based on shape memory alloys is presented based on models developed based on the analysis of the phase transformations in each layer and on their contribution to the stress in the fil-substrate architecture. The analysis of the phenomena associated with the martensitic transformation allows the selection of the alloy composition to obtain a tuneable actuation in the desired temperature range as well as the profile of this operation based on the type of substrate used and its geometry as well as the fabrication parameters. The prediction of a microactuation profile is described for bimorph architectures with a film consisting of one or more shape memory alloy layers.

Keywords: phase transformations, microactuation, shape memory alloys, layered structures.

1. Introduction

Shape memory alloys (SMAs) are recognized as belonging to the category of smart materials as a result of a set of properties, including the shape memory effect, superelasticity, damping capacity, biocompatibility (for some compositions) and even shape recovery in a magnetic field (for certain compositions) [1, 2]. Since their discovery, the peculiar set of properties was analyzed in order to understand the mechanisms behind their functionality and to optimize the outputs [3, 4, 5, 6]. Although SMAs are recognized as metals, the shape memory effect was also

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identified in polymers [7] and even ceramics [8] or gels [9].

From the multitude of functional properties of shape memory alloys, the thermal actuation capacity [e.g.10] is one of the most significant, allowing these materials to be taken into account in the realization of future intelligent structures [11]. They are considered for technical solution in aerospace, structural and biomedical fields [12,13].

The martensitic transformation - thermoelastic, reversible - is the basis of the shape recovery, which occurs after plastic deformation, through heating [14]. The shape recovery is gradual starting at the temperature at which martensite begins to transform into austenite (As) and ends when martensite has transformed into austenite (Af). In the As-Af temperature range, the two phases - austenite and martensite - coexist in a proportion given by the temperature at which the alloy is located. During cooling, although the reverse transformation (from austenite to martensite) takes place in the Ms-Mf interval, a shape change does not occur naturally except after some thermomechanical training treatments [15].

Shape recovery of upon cooling is also possible in the variant in which an association is made between an alloy with shape memory and an element that stores energy during heating into austenite, energy to be used to deform the alloy upon cooling into martensite [16]. In this case, the experimental observation related to the fact that austenite is stiffer, while martensite has a much lower modulus of elasticity, being easily deformed due to the presence of variants in the structure. This possibility to associate an elastic element is used when making two-way actuators, either in massive structures or in structures based on thin films [17].

The advantage of manufacturing actuation elements using the thin film technique lies in the fact that the actuator made of a memory alloy film deposited on a substrate, so as to result in a bimorph structure, is made simultaneously with the incorporated elastic element (usually the substrate) [18,19]. Moreover, due to the fact that the intimate association between the film and the substrate is made at high temperature, a state of tension appears that contributes to the change of shape both during heating and cooling [20].

The possibility of generating actuation structures not only through monolayer but also bi or multi-layer films brings practically unlimited possibilities of modulating the actuation response depending on the temperature of the thus achieved structure.

This work aims to review the possibilities of making simple and complex micro-action structures based on shape memory alloys.

2. Actuation in bimorph structures

Thermal microactuation in bimorph systems is based on the thermoelastic stress generated by the difference in properties between the two components of the bimorph, i.e. the film and the substrate. If, in the case that neither of the two components undergo a phase transformation, only a change proportional to the temperature at which the bimorph is located occurs. In the event that at least one of the components undergoes a phase transformation, a deviation from proportionality occurs as a result of the fact that the phases have different thermoelastic properties. During the phase martensitic transformation one phase gradually transforms into the other one

Table 1 shows the main thermomechanical properties of memory alloys from the Ni-Ti family. The table shows significant differences between the expansion coefficients and Young's moduli of austenite and martensite that can be used to control the stress in bimorph structures with a NiTi SMA film deposited on a substrate made out of a different material. The properties of Si – the mostly used substrate for bimorph microactuators are also shown.

Table 1. Thermomechanic properties of NiTi shape memory alloys and Si, as a usual substrate [21]

Phase / Substrate	**Expansion coefficient** [10^{-6}/°C]	**Thermal conductivity** [W/cm °C]	**Young Modulus** [GPa]	**Poisson Coefficient**
Austenite	11	0.18	83	0.33
Martensite	6.6	0.086	28-41	
Silicon	2.6	1.57	112	0.28

Assuming that the SMA film was deposited at high temperature (necessary for crystallization), during cooling the stress that develops in the bimorph structure causes a cantilever type bimorph actuator to bend towards the substrate or towards the deposited film (depending on the values of the expansion coefficients of the SMA film and of the substrate).

The equipment used for the sputtering was developed in Politehnica University Timisoara and is detailed in Fig. 1a. It allows the magnetron sputtering of thin films (Fig. 1b) out of 2 inch metallic targets under 10 mtorr Ar pressure, using a 100 W power generated by a DC power supply.

The stress recorded in the bimorph materializes through a deflection of the free end of a cantilever type actuator and can be calculated using a version of the Stoney equation. Thus, the stress at the interface of the composite film-substrate cantilever beam is written as:

$$\sigma_f\,(T)= (E_s * t_s^2)\; D(T)/[6R(1-\nu_s)t_f] \qquad (1)$$

where:

σ_f: Stress on the cantilever beam

E_s: Young's modulus of the substrate

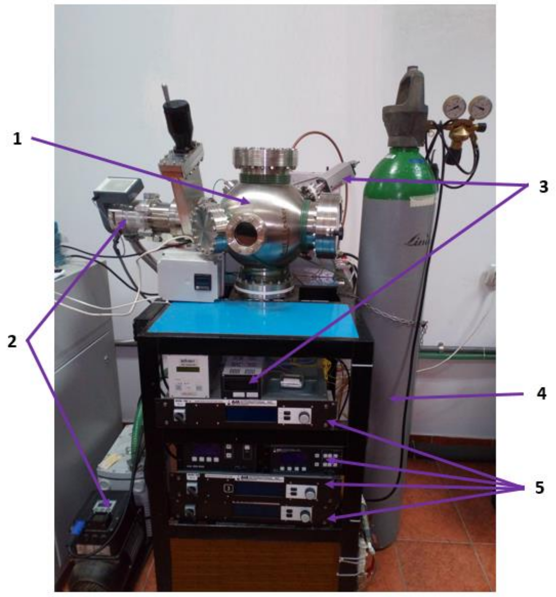
ν_s: Poisson's coefficient of the substrate

t_s: thickness of the substrate

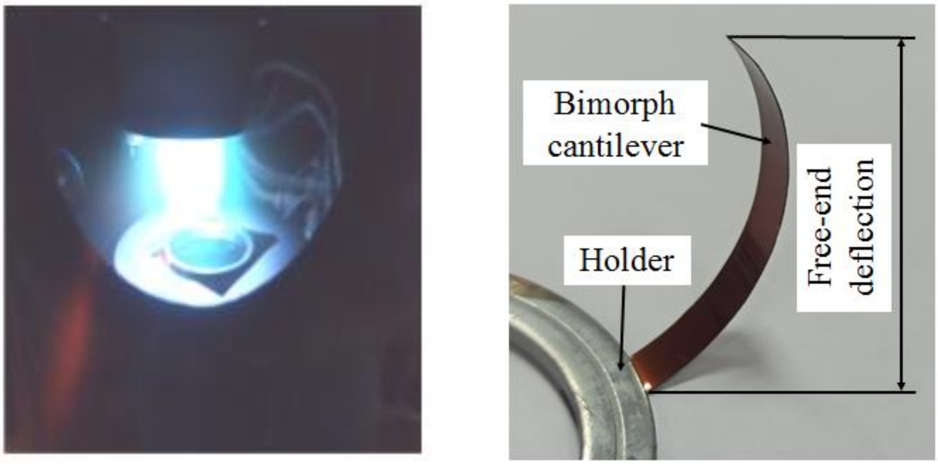
t_f: thickness of the thin film

l: length of the cantilever

D: the deflection of the cantilever



a. DC Magnetron sputtering equipment designed and assembled in Politehnica University Timisoara (1 – sputtering chamber, 2 – vacuum pumps, 3 – vacuum measurements system, 4 – Ar gas, 5 – DC power supplies).



b. NiTi film sputtering on substrate

c. example of cantilever bending

Fig. 1 Experimental details concerning the film sputtering.

When deflection of the cantilever is not too high (D<<l), σ_f can be written as:

$$\sigma_f\,(T) = (E_s \cdot t_s^2) D(T) / [3 \cdot l^2\,(1-\nu_s)\,t_f] \qquad (2)$$

A typical stress vs. temperature curve determined by experimentally measuring the deflection of the free end of a cantilever-type bimorph during the thermal cycling is shown in Fig. 2.

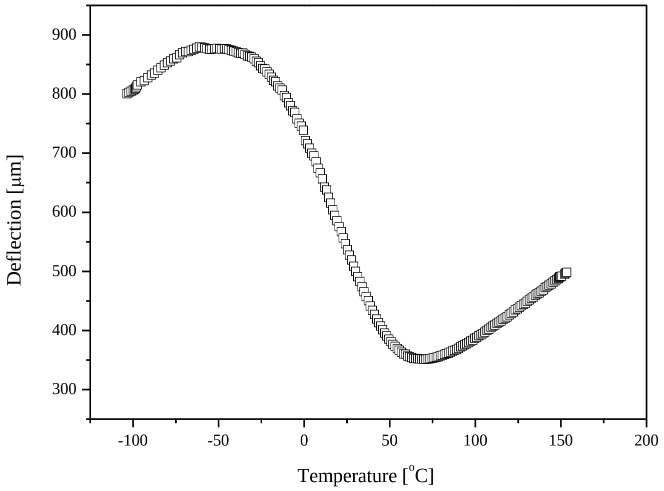


Fig. 2. Typical deflection vs. temperature curve determined for a bimorph with single layer NiTi SMA film magnetron sputter-deposited on a Si substrate.

The analysis of the data in Fig. 2 allows highlighting the effects of the martensitic transformation in the shape memory alloy film, and the effect of this transformation on the tension in the film, on each temperature segment (before the transformation, during the transformation and after its completion) as highlighted in Fig. 3.

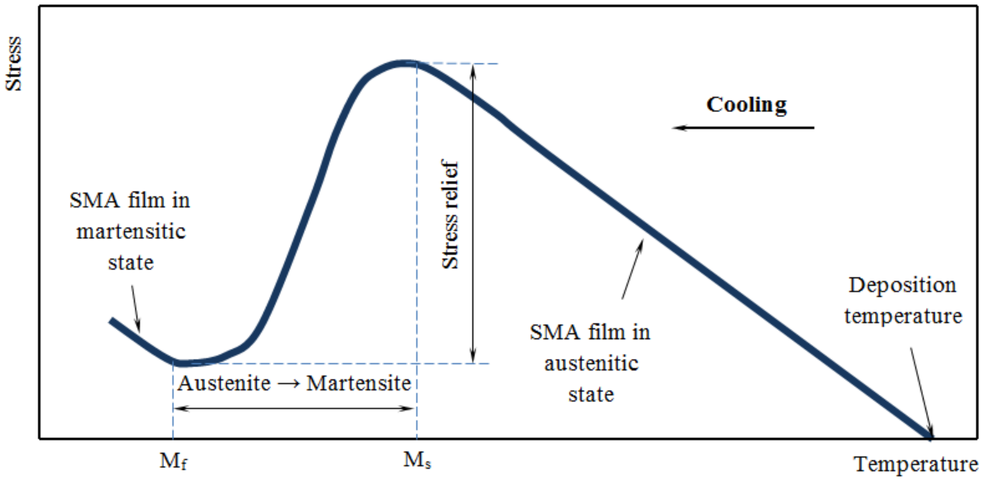


Fig. 3. Stress analysis on cooling in bimorphs generated by deposition the SMA film on heated substrates.

3. Prediction of actuation in layered SMA-based structures

The issue of microactuation with shape memory alloys becomes more complex when layered structures are considered. From the analysis related to Fig. 3 it follows that if the shape memory alloy film is deposited at a lower temperature its stress relief is reduced compared to the case in which the stress accumulation on cooling from the deposition temperature is higher at the onset of the martensitic phase transformation. Thus, assuming that the shape memory alloy film that is part of a bimorph structure is composed of two layers deposited at different temperatures, each layer will have its own contribution to the stress relief during its phase transformation. This is observation is in principle reflected in Fig. 4.

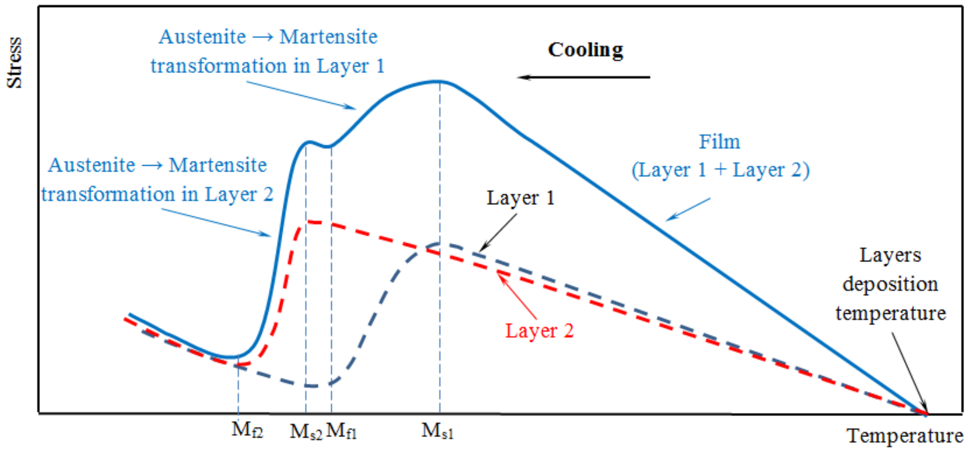


Fig. 4. Stress analysis in a double layer Ni-Ti-based SMA film deposited on Si substrate.

Assuming that the double layer film (composed of a layer with a transformation at a higher temperature compared to the other layer) is deposited at high temperature, it can be seen from Fig. 4 that the composed stress on cooling of the bimorph with a SMA bilayer will follow the conventional bimetal stress vs temperature path until it reaches the temperature at which the first transformation occurs in layer 1. In this point a stress relief then starts in the bilayer film due to the austenite-martensite transformation in the layer 1 that is slightly counterbalanced by the stress increase due to the further cooling of the austenite in layer 2. The situation continues until the austenite-martensite transformation initiates in the second layer and from this point forward – assuming that both films are in the temperature range of their transformations, the stress relief continues at a steeper rate. Once one of the layers ends its transformation into martensite, the stress in that layer starts to increases and contributes to the overall stress in the film.

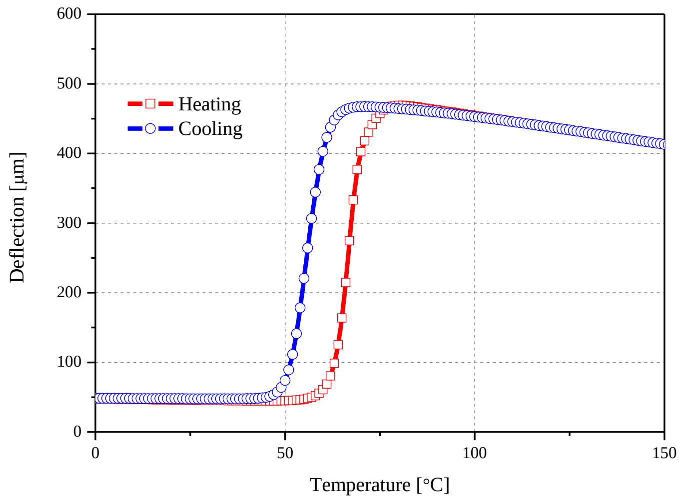
Based on the above detailed approach, it becomes possible to design microactuators in which the deflection vs temperature profile can be tuned based on the difference between the phase transformations in each layer.

Using this principle, our model developed for layered structures [22] can be used to generate predictions on the actuation profile of bimorphs with layered films. The set of simulations using the model developed for multi-layered films, is detailed for the case of single layer, bilayer and trilayer microactuators with NiTi SMA films deposited on Si substrates, with the simulation parameters described in Table 2 and figures 5a-c.

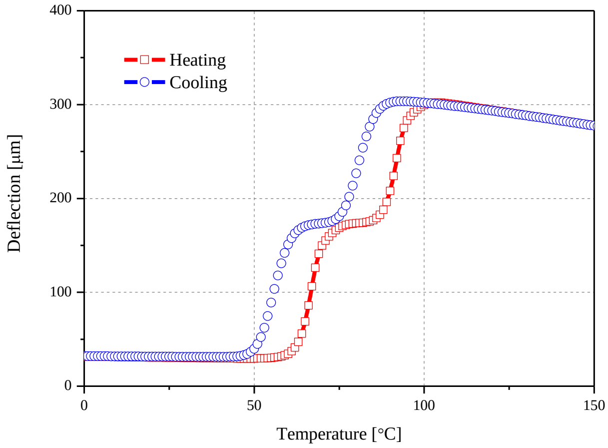
Table 2. Parameters for NiTi/Si cantilever-type microactuators used in the simulation

Cantilever microactuator type	**Substrate thickness** [µm]	**Layer 1**		**Layer 2**		**Layer 3**		**Fig.**
		Thickness [µm]	Ms [°C]	Thickness [µm]	Ms [°C]	Thickness [µm]	Ms [°C]	
Single layer	100	1	60	-	-	-	-	**5a**
Bilayer		0.5	60	0.5	80	-	-	**5b**
Trilayer		0.333	60	0.333	20	0.333	-20	**5c**
All films deposited at the same temperature								

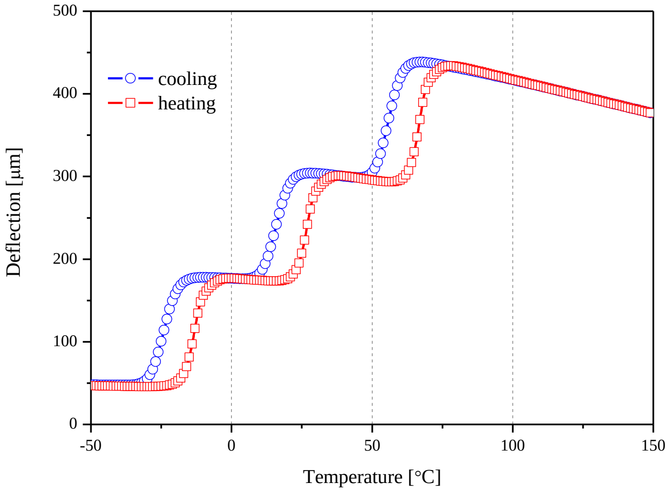
Compared to bimorph microactuators with homogeneous films (fig. 5, a) it can be seen from Figs. 5, b, c that it becomes possible to modulate the microactuation either by extending the temperature range over which the actuator maintains a certain position and/or to generate one or more actuation plateaus in which the deflection of the cantilever-type bimorph microactuator maintains a fixed position.



a. Single layer SMA film.



b. Bi-layered SMA film with equally spaced transformation temperatures of the layers.



c. Tri-layer film with equally spaced transformation temperatures of the layers.

Fig. 5. Deflection vs. temperature simulations for bimorph structures with shape memory alloy film deposited on a non-transforming substrate.

4. Conclusions

The realization of micro-acting elements based on thin films is possible using the sputtering of shape memory alloys on a substrate. For cantilever-type microactuators, the actuation range mainly depends on the thermomechanical properties (Young modulus and thermal expansion coefficient) of the film and the substrate, the deposition temperature and the geometrical aspects of the film/substrate cantilever.

For a 1µm NiTi film on 20 mm long/100 µm Si substrate, deposited at 600˚C, the actuation can reach up to 6-800 µm, depending of the transformation temperature of the film. The reproducibility of the date for bimorph structures is substantially better than the one of actuators based only on shape memory alloy films (unconnected to the substrate), due to the elastic connection that provides a controllable shape recovery not only on heating, but also on cooling.

The advantages of bimorph structures made in this way reside in:

- simultaneous generation of the structure (film+substrate) by sputtering.
- obtaining a double shape memory effect in the substrate film system, so that when martensite transforms into austenite, the shape of the microactuator changes in one direction, while upon cooling, the transformation of austenite into martensite leads to a shape change in the opposite direction.
- control of transformation temperatures and transformation hysteresis is achieved by controlling the composition of the alloy film with shape memory. The greater the difference between the temperature of making the bimorph with a crystalline film of the memory alloy and the temperature at which the martensitic transformation occurs, the greater the microactuation effect.
- the main elements that are used in the selection of the components of a bimorph microactuator based on shape memory alloy film are the composition of the shape memory alloy and the material of the substrate. Their properties (module of elasticity and coefficient of expansion) influence the ability of micro-action.
- the generation of the multi-layer memory alloy film allows the response of the microactuator to be modulated over a temperature-controlled interval, so that it can meet the requirements of a specific application.

The development of microactuators based on alloys with shape memory allows expanding the range of microelectromechanical systems based on elements with high actuation capacity.

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