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Biomechanically Inspired Shape Memory Effect Machines Driven by Muscle Like Acting NiTi Alloys

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Abstract: The research shows a bioinspired approach to be adopted to design of systems based on Shape Memory Alloys (SMAs), a class of Smart Materials that has in common with muscles the capability to react to an impulse (thermal for SMAs) with a contraction. The biomechanically inspired machine that is discussed in the paper refers to the antagonistic muscles pairs, which belongs to the Skeletal Muscles and are normally arranged in opposition so that as one group of muscles contract another group relaxes or lengthens. The study proposes a model, a solution not only to design a specific application, but also to provide an approach to be used for a wide range of adaptive applications (switchable windows, smart shadow systems, parking and urban shelters, etc.), where the shape changes in response to different external stimuli. The use of antagonist pairs mechanism provides a solution for better optimized systems based on SMAs where the main and proven advantages are: Easier and faster change of shape, lower need of energy for system operation, lower cost for SMA training and no problem of overheating.

Keywords: Smart Factory, Centrifugal Pipe, Process Control, Glass Reinforced Plastics, Chemo-Rheology

Introduction

The research presented has the aim to show that better optimized systems based on Shape Memory Alloys (SMAs) can be designed using muscles working as biomimetic model. In particular the Skeletal muscles and the antagonistic pairs have been used as biomechanical model, they are the voluntary muscles that allow the body to move and they make up 40% of an organism's body mass (Lindstedt, 2016).

Skeletal muscles are held to the bones by tendons, which role is to transfer the force generated by the muscles contraction to the bone joint. Tendons are made of robust tissue and they work as special viscoelastic connectors between bone and muscle. For an adduction movement in a joint, contraction and shortening of the muscle generates a force that is applied on a lever system that causes the joint adduction movements. To recover its initial position, the reciprocal muscle on the other side of the joint contracts and shortens. As described by Biewener and Roberts (2000), muscles are normally coupled in opposition so that movements of joints are driven by a mechanism in which one group of muscles contracts while another group relaxes or lengthens.

Basically antagonistic pairs are muscles where one moves the bone in one direction and the other moves it back the other way in transmission of nerve impulses to the muscles. In the adduction movement of a human arm, the agonist biceps shortens and bends the forearm on the elbow joint, conversely, on arm abduction movement; the antagonist triceps shortens and returns the forearm to its original position. In general, the muscle that applies the force needed for a movement is only one of agonist-antagonistic pairs and, in particular, there is always a selective stimulation driven by the brain that acts on the muscle that contracts or shortens (agonist), while the behaviour of the reciprocal is passive, it works roughly like a brake (antagonist). The active muscle for a specific movement is always the one that contracts (Yang *et al*., 2013).

A unique class of Smart Materials that has in common with muscles the capability to react to an impulse (thermal in this case) with a change of shape and thus also with a contracting movement if necessary is that of Shape Memory Alloys (Van Humbeeck, 2010; Meisel *et al*., 2014; Melton and Mercier, 1980).

This analogy between muscles contraction and extension and the ability of this class of intermetallic alloys to undergo contraction and extension (superelasticity) under the effect of thermal and mechanical stimulation, allow us to derive a biomechanically inspired machine based on these materials.

U.S. Naval Ordnance Laboratory discovered shape Memory Effect for the first time during 1960s. The researcher of the Laboratory found this effect in a 1 to 1 alloy of Nickel and Titanium, but only nowadays, a higher spread for biomedical field, actuators, couplings and surgical instruments. Anyhow, applications of SMAs for industrial or product design are still so poorly spread and SMAs potentialities are only rarely and weakly exploited.

Nickel-Titanium alloys are intermetallic compounds (Otsuka and Ren, 1999) and they able to show thermal shape memory effect, namely, to return to their original shape on heating even when largely deformed (up to 10%).

The Stress-Strain-Temperature diagram of Fig. 1 resumes the thermo-mechanical behaviour of these NiTi based materials.

The NiTi alloy assumes, at higher temperatures, an interpenetrating simple body centred cubic structure known as Austenite (Meisel *et al*., 2014).

When brought at lower temperatures (treatment A in Fig. 1 and 2), this intermetallic alloy freely solid-solid transforms to a constrained and more complex face-centred tetragonal crystalline structure identified as Martensite.

The Body-Centred Cubic (BCC) crystal structure of Austenite (Xiangyang *et al*., 2003) shows only one possible crystallographic habit that can be got at equilibrium (high temperatures state 1 in Fig. 1) that is identified as B2 type (Fig. 2). On cooling, Austenite crystals undergo a constrained solid-solid diffusionless transformation to metastable Martensite. After Otsuka and Ren (1999) it has been recognized that, in binary TiNi transformation proceeds from the parent BCC structure (B2 type in Fig. 2) to martensitic FCC lattices. The body-centred cubic parent austenitic phase (B2) may transform by a diffusionless local shear mechanism into an orthorhombic or monoclinic martensite phases. The later martensite lattice is a monoclinic B19′ phase (Otsuka *et al*., 1971; Knowles and Smith, 1981; Miyazaki *et al*., 1984; Matsumoto *et al*., 1987), which has been justified as a monoclinic alteration of the B19 orthorhombic structure (Fig. 2).

The transition amongst these structures needs small thermal activation because involves diffusionless transformation and easily results in the restrained and rapid rearrangement of atomic positions.

For this crystalline conformation, however, two differently oriented crystallographic variants with small energetic differences exist. These two configurations consist of the twinned (B19 in Fig. 2) and detwinned (B19' in Fig. 2) rearrangements of atomic planes without crystal plane slip (states 2 and 6 of Fig. 1). Due to thermodynamic considerations, the twinned structure freely occurs in unstressed conditions (state 2).

The Martensite is described to be crystallographically reversible, which involves that a given plate undergo a backward reverse shear upon heating.

Normally, the Martensite forms, on cooling, only under M_s, however, it could even occur at temperatures higher than Ms if a stress is applied (Yang and Wayman, 1999).

The Martensite formed in these conditions is named Stress-Induced Martensite (SIM).

It can be deduced that the prevailing driving force for Martensitic transformation above M_s is not thermal but mechanical (transformations B in Fig. 1 and 2). Above the temperature where Martensitic transformation starts (Ms), the stress required to produce SIM progressively increases with increasing temperature (Šittner *et al*., 2014).

The linear variation of stress to induce Martensite as a function of temperature has been experimentally observed and it can be also derived through a thermodynamic approach. The thermodynamic governing the relationships between physical properties (volume, temperature, pressure) variations obeys the Clausius-Clayperon equation and is written as:

$$\frac{dP}{dT} = \frac{\Delta H}{T \cdot \Delta V} \tag{1}$$

where, P is the pressure, T is the temperature and ΔH is the latent heat of phase change (that can be determined by DSC analysis) and ΔV is the volume change of the phase change (the volume change for NiTi Austenitic to Martensitic phases may be calculated from the dimension of the crystalline units, namely a cube of 0.3015 nm for Austenite to the 0.4622×0.4120×0.3015 nm for the Martenisite (orthotrombic or nonoclinic).

Equation 1 that may result more convenient in chemical physical and chemical fields but for mechanical aspects it may be substituted by a Clausius-Clayperon derivation (Duerig *et al*., 1990) that assumes the form:

$$\frac{d\sigma}{dM_s} = -\frac{\Delta H}{T \cdot \varepsilon_0} \tag{2}$$

where, ΔH and T have the same interpretation as for Equation 2 and σ, M_s and ε_0 are the applied stress, the shifted Ms temperature and the transformational strain resolved along the direction of the applied stress.

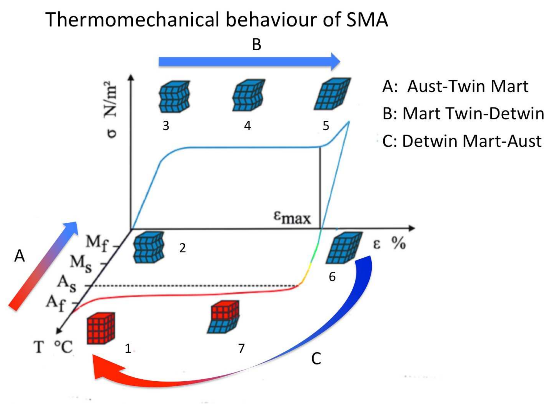

Fig. 1. SST diagram of thermal and mechanical induced transition in Shape Memory Alloys

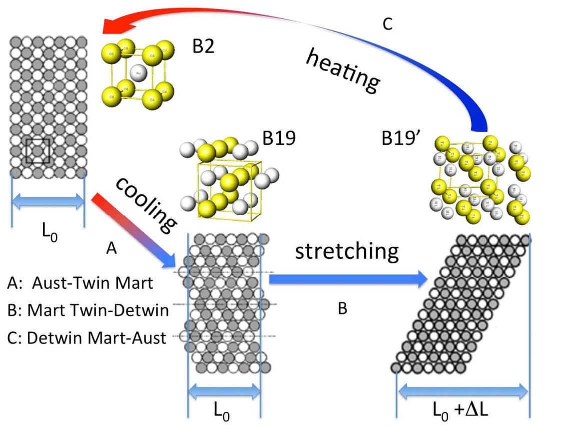

Fig. 2. Thermal and mechanical induced transition in Shape Memory Alloys

Moreover, it has been theoretically predicted (Clasius Claypeiron Equation 2) and experimentally determined (Šittner *et al*., 2014) that the level of mechanical loading necessary to create Stress Induced Martensite (SIM) growths linearly with temperature. These reversible solid-state phase transformations are known as a martensitic transformation that requires to occur, depending on temperature, mechanical loading stresses between 70 to 140 MPa (Duerig *et al*., 1990).

According to Equation 2 the stress drops to zero at the temperature M_s.

The difficulty to stress induce Martensite continues to increase with temperature until M_d, above which the critical stress required to induce Martensite is greater than the stress required to move the dislocations (not reversible plastic deformation).

Therefore the temperature range for SIM is from M_s to M_d. For a number of SMA systems, the agreement in the temperature dependence of the stress to form SIM according to the Clausius-Clayperon equation is quite striking.

The equation works equally well for the non-isothermal case, i.e., the case where temperature was held constant while the stress needed to form Martensite was measured.

Super-elasticity occurs when a material is deformed above A_s, but still below M_d. In this range, Martensite could be stabilized with the application of stress, but becomes unstable upon removal of stress.

By mechanical stretching (treatment B in Fig. 1 and 2), in fact, the SMA is deformed to a larger extent (states 3 to 4 in Fig. 1 and structures B19 and B19' in Fig. 2). This pseudo-plastic deformation is enabled by reorientation of crystallographic variants in the cold temperature phase following twinned (B19) to de-twinned (B19') martensite transformations. Consequently, the deformation persists after load removal (from state 2 to 3 in Fig. 1). On re-heating, process C in Fig. 1 and 2, the material progressively transforms to Austenite B2 crystal lattice (from state 6 to intermediate state 7 and final state 1 in Fig. 1) recovering its initial shape.

During this shape recovery, large strain changes and large forces are generated that are of particular benefit for the development of temperature-activated actuators.

As reported on the temperature axis of Fig. 1, the four characteristic temperatures of SMAs are M_f (Martensite finish), M_s (Martensite start) on cooling and A_s (Austenite start) and A_f (Austenite finish) on heating.

When SMA is heated, it starts to change into Austenite phase at A_s and it completes the transition at A_f temperature; similarly, on cooling, it starts the transformation to Martensite at M_s temperature and it completes the transition at M_f temperature.

However, for some NiTi alloy compositions, an intermediate phase, called R-phase with rhombohedral structure, could also manifest, in this case the characteristics temperatures are indicated as R_s and R_f. This event manifests itself by thermal events that can be measured in Differential scanning Calorimetry. The calorimetric analysis has been run on our samples to identify not only austenitic than martensitic characteristic temperatures but also the occurrence of the intermediate rhombohedral lattices.

The SMAs can exhibit two kind of Shape Memory Effect (SME), defined as one-way and two-way effects. For one-way effect we mean the SMAs ability to remember and resume the macroscopic shape associated with austenitic phase when heated up to A_f temperature; for two-way effect, instead, we mean the first ability described added to the capability to recover also the macroscopic shape associated with martensitic phase when cooled up to M_f temperature.

To get one or two-way memory effect, in order to program pre-set shapes for martensitic and austenitic phases, thermo-mechanical treatments are required (Naresh *et al*., 2016).

The basic idea of this paper on how and why to use the biomechanical model of muscles working is discussed in the next paragraphs.

Materials and Methods

Materials

In order to experiment and develop the biomimetic model aimed to the optimization of systems based on SMAs wires Dinalloy Inc.

Flexinol is a SMA with Nickel and Titanium as main chemical constituents.

Apparatus and Procedures

Differential Scanning Calorimetry (DSC)

Thermocalorimetric analyses have been carried out on NiTi alloys. The DSC technique determines the temperature and the heat flows associated with material transitions as a function of time and temperature. It also provides quantitative data on endothermic (heat absorption) and exothermic (heat evolution) processes of materials during physical transitions (Ziólkowski, 2012; Shaw *et al*., 2008).

The thermocalorimetric characterization has been carried out in a nitrogen atmosphere by a Mettler ADSC Differential Scanning Calorimeter equipped with a liquid nitrogen cooling unit in the range of temperatures between -30 and 120°C. Temperature scans were carried out at 5°C/min. For sample stabilization, isothermal scan were run at 500°C, heat flux were recorded up the final apparent equilibrium (heat flux = 0). The high temperature treatment induces the crystal structure atoms to re-arrange into the most compact and regular pattern possible finally resulting in a rigid cubic austenite phase (Kauffman and Mayo, 1993). A typical DSC thermogram performed on a specimen of Flexinol wire (0.25 mm of diameter, 4,00 mg) has been reported in Fig. 3.

Results and Discussion

For the SMA alloy of our work, a dynamic test composed by one heating segment from -30 to 120°C and one cooling segment from 120 to -30°C and with a rate for temperature change of 10°C per min have been carried out and it is reported in Fig. 3.

The thermal analysis have been performed after an isothermal treatment at 500°C, used to simulate the condition needed (annealing) for SMA training, in order to "memorize" its austenitic shape. This step is important because the suppliers of SMAs provide only information on characteristic temperatures that the alloy has before of its training, but the range of transition temperatures changes after the heat treatment used for SMA programming (Kus and Breczko, 2010). The apparatus utilized for thermal analysis was a ADSC Mettler Toledo.

The DSC traces in Fig. 3 reports the thermograms on heating (lower part) and cooling (upper part) relative to the SMA investigated. All SMA samples were, as previously stated, heat-treated for 10 min at 500°C in order to stabilize the Austenitic phase.

The first heating cycle run at 10°C/min, shows the endothermic peak of the Martensitic-Austenitic transition (lower part of Fig. 3). The orthorhombic martensite (B19) phase transformation into the body-centred cubic parent austenitic phase (B2) starts at 49°C and ends at 60°C (dotted lines in Fig. 3).

The cooling part of the thermic cycle shows a more complex thermal behaviour. Two peaks were observed on cooling.

The B19′ monoclinic Martensite, in fact, can be obtained either by a single step phase change of B2 → B19′ (a single peak in the DSC), or by a two-step phase change of B2 → R-phase → B19′ (Otsuka and Ren, 1999; Otsuka *et al*., 1976; Yang and Wayman, 1992a; 1992b) and two peaks will be evident on a DSC thermogram.

In the two-step transformation, the R-phase is an intermediate rhombohedral phase that is not compatible with the final cubic B2 austenitic phase. The lattice parameters of B2 phase, R-phase and B19′ phase and the correspondences between the B2 to R-phase and B2 to B19′ lattices transitions, have been well established (Otsuka *et al*., 1971; Knowles and Smith, 1981; Matsumoto *et al*., 1987; Yang and Wayman, 1992a; 1992b).

The two step transformations of B2 → R-phase and sub- sequent R-phase → B19′ may occur upon cooling when Rs (the start temperature of B2 → R-phase transition) is above Ms (start temperature of martensite transformation) (Otsuka and Ren, 1999). This phenomenon was also observed in stress-induced transformations (Otsuka *et al*., 1976).

The differential thermal and the stress-strain treatments of Fig. 2 characterize the temperature-induced and stress-induced two-step transitions in an alloy of NiTi, respectively.

Figure 4 reports a detail of the DSC thermograms relative to this double stage transition observed on the cooling thermogram.

Upon cooling the parent phase B2 transfers first to rhombohedral phase (R-phase) and then, at R_s, from R-phase to martensitic phase at M_s, finally the martensitic transformation from R-phase is completed at M_f. The reverse transformation occurs from martensitic phase directly to the parent phase B2 at A_s and is completed at A_f. (at temperature near -10°C).

On the same Fig. 4 (upper part) it has been also reported an experimental curve on the temperature dependence of the Martensite start Ms on Ni-Ti relative composition given either in Nickel content (left axis) and Ni-Ti ratio (right axis) derived from Harrison and Hodgson (1975) and Hanlon *et al*. (1967) data.

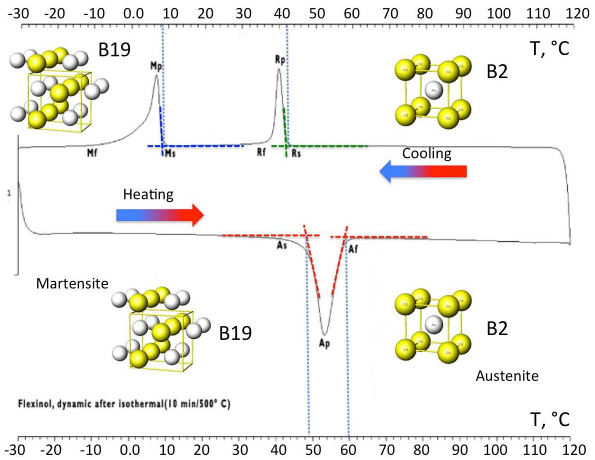

Fig. 3. DSC analysis performed for a specimen of Flexinol wire. Heating segment from -30 to 120°C, cooling segment from 120 to -30°C. Heating and cooling rates 10°C/min

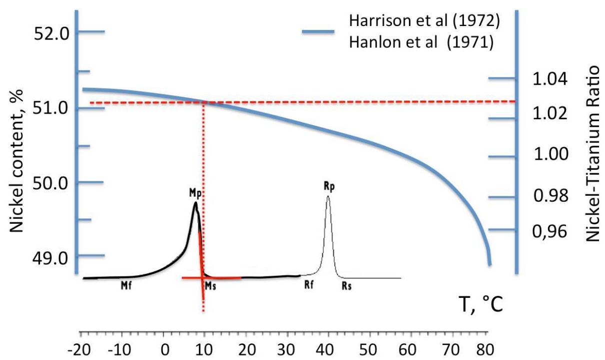

Fig. 4. Detail of DSC characterization of the NiTi alloy composition in the cooling stage

From our thermal characterization, a composition of 51% Ni content (1.03 Ni-Ti ratio) has been observed (dotted red line in Fig. 4).

Huang *et al*. (2003) have given a physical explanation that eliminated the need for two different mechanisms to describe the two-way shape-memory effect.

They have found that the B19′ structure of NiTi is not stable in his base-centred orthorhombic structure and that it cannot store at the atomic level shape memory effect. Nevertheless, this structure has been described to be stabilized by a wide range of residual internal and applied stresses and that the shape memory is stored primarily at the micro-structural level.

The use of muscle working model depends also on the necessity to optimize the systems based on SMAs by the point of view of their energy need and not only for their ability to change shape.

Due to the quite low temperatures for martensitic transition (M_f, -10°C), in order to use a SMA programmed for a two-way shape memory effect in an industrial application, the machine should be equipped of a cooling system to get the Martensitic phase transition and to hold it, on the other hand the need of a heating system to get and hold the Austenitic crystal phase. The kind of system developed is based on the use of SMA wires trained to have a one-way SME and, thus, to "remember" only the pre-set shape associated with austenitic phase. The movements and, thus, the changes of shape depend only on the forces generated by the wire contracting like the antagonistic pairs mechanism existing for the muscles.

Basically the system is composed by hinge joints and a lever mechanism assembled to SMA wires. When the wire (SMA adductor blue line in the middle of the machine reported in Fig. 5) shortens, it pulls and causes through hinge joints and lever mechanism the change of shape (adduction of the two parts of the moving systems). To return the system to its original position (abduction), the "reciprocal" external wires on the sides of the joint (red lines in Fig. 5) must contract and shorten.

Similarly to work of the muscle, when the wire in the middle contracts, the others stretch and lengthen and vice versa.

The wires contraction can be selectively activated by electrical current passage that causes an increase of the wire temperature (due to its electrical resistance and, therefore, their heating (Sofla *et al*., 2008).

A schematic representation of the biomechanically inspired machine is reported in Fig. 6.

The solution is possible by the mechanical point of view and affordable referring to the forces generated by the wire. In fact, the characteristic mechanical properties of SMAs, depends on the crystal phase and, thus, for different temperature ranges the mechanical behaviour is different.

In particular, the Young's Modulus of austenitic phase can be several times higher than that of martensitic phase.

For this reason SMAs are easier to strain at low temperature (martensitic range of temperature) than at high temperature (austenitic range of temperature). The forces generated, instead, because of the different value of Young's Modulus during the thermal-induced change of shape associated with austenitic B2 phase are higher than for twinned martensitic B19' phase (Melton and Mercier, 1980).

The force generated in our NiTi alloy wire of 0.51 mm for Martensite B19' to Austenite B2 transformation is almost 250% higher than for twinned B19 Martensite to the detwinned B19' Martensite (Dynalloy technical sheet).

Namely, the pull force on heating contraction (lower part of Fig. 6) is 34.92 N and once cooled from the underformed B19 to B19' detwinned strained Martensite force is 13.96 N (upper part of Fig. 6).

This thermo-mechanical SMA effect may be used to mimics biomechanical behaviour of agonist and antagonist muscled to precisely drive a bio-inspired machine.

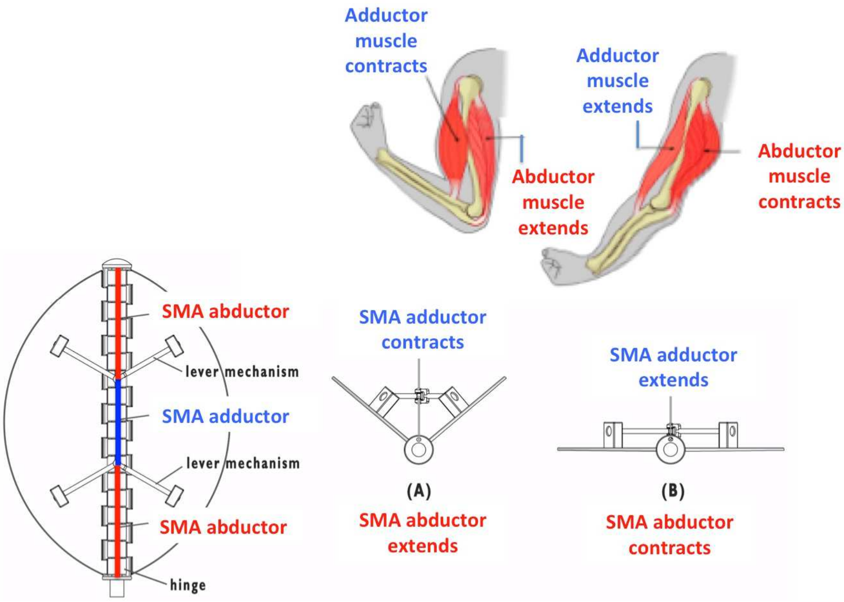

Fig. 5. Biomechanically inspired SMA driven machine

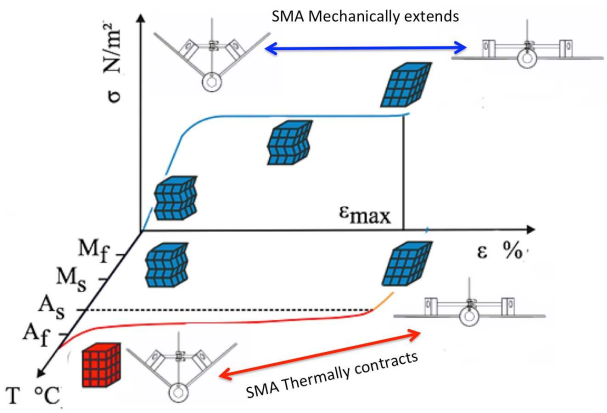

Fig. 6. Thermo-mechanical transformations of SMA adductor and abductor of the biomechanically inspired machine

As indicated in Fig. 6, where the thermo-mechanical NiTi alloys behaviour and the bio-inspired machine of Fig. 5 are reported, the heated SMA agonist thermal contraction, which is associated to the detwinned Martensite B19' to Austenitic B2 transformation, produces the adduction of the two machine arms, meanwhile the SMA abductor extends passing from B19 twinned Martensite to stretched detwinned B19' Martensite (A in Fig. 5).

The machine arms extension can be, conversely, obtained by inverting the heating-stretching signal (B in Fig. 5). In this movement the previously extended SMA abductor contract from B19' detwinned Martensite to B2 Austenite while the SMA adductor extends from twinned B19 to detwinned B19' Martensite.

Conclusion

A system that exploits the above-mentioned mechanism can be used, in general, for industrial applications characterized by a smart and responsive behaviour. The aim of the research presented is not to design a specific application, but to provide a biomimetic model to be used for a wide range of adaptive applications (switchable windows, smart shadow systems, parking and urban shelters, etc.), where the shape changes in response to different external stimuli.

Some advantages connected to the use of the biomimetic model of muscle working are discussed in more detail in the next paragraph.

The main advantages connected to the biomimetic approach described in the previous paragraph are:

- Easier and faster change of shape
- Lower need of energy for system operation
- Lower cost for SMA training
- No problem of overheating

To better understand the advantages listed, it is important to underline that a SMA trained for one-way effect, when heated up to A_f takes the macroscopic shape associated with austenite and then, cooling down, altough there is a change of crystal phase it retains the macroscopic shape of austenitic phase(if no loads are applied). Differently, if the SMA has been trained for a two-way effect, when it cools down, changes its shape taking the shape associated with martensite.

A problem of two-way effect is that it is easy and fast to heat the SMA by electrical current, but the cooling time (if no external and appropriate devices are used) is quite high and depends on room temperature and on geometry of SMA. Our SMA wire with a diameter of 0.51 mm and a current of 4 A takes 1 sec to contract (austenite) but roughly 17 sec to cool down to 70°C (considering a room temperature in static air) (Dynalloy technical sheet). Heating and cooling times are strongly dependent on many factors (current, chemical composition, geometry and thickness of SMA, room temperature, presence of cooling systems, etc.). Anyhow it is enough to show the large difference between the times needed to heat and cool a SMA wire.

The system developed, using wires that only contracts (antagonistic pairs mechanism), gives a faster change of shape. Moreover, since with one-way SME the wire retains the macroscopic shape associated with austenitic phase also when it cools down, there is not the need to hold austenitic range of temperatures and, thus, the use of current is only necessary for few seconds. Consequently, the need of energy for system operation is so much lower. If we suppose, for example, to use two SMA wires, one with a one-way effect and another with a two-way effect, with a diameter of 0.51 mm for 1 h per day for 1 month in their austenitic phase, since we need 4 A in the first case for 1 sec (per day) and in the second case for 3.600 sec (per day) and we consider to apply a voltage of 6 V. Using simple calculations:

$$P(W) = I(A) \times V(V)$$
$$E(kWh/month) = P(W) \times t(h/day)/1000(W/kW) \times 30$$

In the first case we have an energy consumption (E) of 0.0001 kWh/month and in the second of 0.7200 kWh/month (Technical sheet Dynalloy).

Moreover, using one-way effect and, thus, avoiding heating for a long time a SMA wire, there is no overheating. If a SMA is overheated, there is a degradation of its properties (Velázquez and Pissaloux, 2012).

Finally, also the training of SMA with one-way effect become easier and cheaper, in fact, the treatment requested to set the austenitic shape is composed only by one step, instead, two-way training (SME or SIM training procedures) needs thermo-mechanical treatments that must be repeated 20-30 times (Lahoz and Puértolas, 2004).

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Author's Contributions

All the authors contributed equally to prepare, develop and carry out this manuscript.

Ethics

This article is original and contains unpublished material. The corresponding author approved the manuscript and confirms that no ethical issues involved. Authors declare that are not ethical issues and no conflict of interest that may arise after the publication of this manuscript.

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