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Using shape memory alloys: a dynamic data driven approach

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Abstract

Shape Memory Alloys (SMAs) are capable of changing their crystallographic structure due to changes of either stress or temperature. SMAs are used in a number of aerospace devices and are required in some devices in exotic environments. We are developing dynamic data driven application system (DDDAS) tools to monitor and change SMAs in real time for delivering payloads by aerospace vehicles. We must be able to turn on and off the sensors and heating units, change the stress on the SMA, monitor on-line data streams, change scales based on incoming data, and control what type of data is generated. The application must have the capability to be run and steered remotely as an unmanned feedback control loop.

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1. Introduction

We describe an ongoing research project to develop a dynamic data driven application system (DDDAS) for porous Shape Memory Alloys [1] using multiscale methods and finite element methods. This paper is a continuation of a paper introducing our research [2]. We use a virtual shaker device for experimentation in order to determine how many sensors are appropriate overall as well as at any given time, how the sensors influence the models, and how to dynamically set the sampling rate.

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Shape memory alloys (SMAs) and porous shape memory alloys (pSMAs) are alloys that remember shapes that can be recovered by controlling the temperature and stress. The difference between a SMA and a pSMA is that SMAs are solid and pSMAs are porous. Both are made from alloys that can shift their crystal structure under repeatable conditions. They are usually Joule heated using an electrical source. Ferromagnetic SMAs (FSMAs) are another class that change shape based on magnetism, which is faster than using heat alone.

Most metals do not show a shape memory effect even if they can have different crystal structures. SMAs can revert to their original shape after heating since their crystal transformation is fully reversible. In standard crystal transformations the atoms in the structure travel through the metal using a diffusion process. This changes the composition locally while the metal as a unit is composed of the same atoms. A reversible transformation does not involve this diffusion of atoms. Instead all the atoms shift simultaneously to form a new structure. A geometric motivation is a parallelogram can be made out of a square by pushing on two opposing sides. At different temperatures, different structures are preferred. When the structure is cooled through the transition temperature the Martensitic structure forms from the Austenitic phase.

SMAs have been known since 1932 when Ölander discovered the pseudoelastic behavior when heating a Au-Cd alloy [3]. The transformation under cooling is pseudoplastic behaviour. The formation and disappearance of a Martensitic phase by decreasing and increasing the temperature of a Cu-Zn alloy was observed in 1938. The basic phenomenon of the memory effect governed by the thermoelastic behavior of the martensite phase was reported in the late 1940's and early 1950's. The first commercially successful material, nickel-titanium alloys or Nitinol, was developed in the 1960's at the Naval Ordnance Research Laboratory and first used in 1970 in the F-14 Tomcat fighter plane.

SMAs are cast using vacuum arc melting or induction melting, which are specialist techniques used to minimize impurities in the alloy and keep the metals well mixed. The resulting ingot is typically hot rolled into longer sections and then diced. Training the alloys is subjective to what properties are desired and shapes that must be remembered. Training requires heating the alloy so that the dislocations reorder into stable positions while cool enough that the alloy does not recrystallize. SMAs are typically heated for about 30 minutes to between 400 °C and 500 °C. SMAs are shaped while hot and then cooled rapidly by quenching in water or air cooled.

In some respects, SMAs are a successor to tempered materials, e.g., steel. Since approximately 1200 BCE civilizations in Europe, Asia, and Africa have known how to make tempered steel. Pickaxes and swords are common early examples. In recent centuries, well known Dark and Middle Ages corporations (e.g., Wilkerson or Krupp Industries) have adapted to the loss of the sword business by transferring their techniques to common consumer products like razor blades and general steel products for construction.

Changing shapes is not instantaneous nor is the response time symmetrical shifting back and forth between different shapes. One of the desired shapes may take seconds to configure using Joule heat. To get back to the default shape usually takes longer since cooling is required. In fact, five to ten times longer is common. Porous SMAs using an appropriately cold liquid is one of the approaches to reduce the response time to restore the default shape.

Another approach (“lagged”) to reducing the response time is to encoat the SMA in a conductive paste within a compliant shell. The heating process can be enhanced and one way in the shape change can be done faster than with just heating the SMA. The cooling time is still an issue.

SMAs have a limited life span due to naturally occurring fatigue in the alloy. Micro scale crystal breaks occur over time reducing the effectiveness of a SMA device. Heating and cooling also causes breaks. Being able to measure that a SMA device is no longer reaching exactly its expected shapes and by how much will allow for better monitoring when a SMA device needs to be replaced.

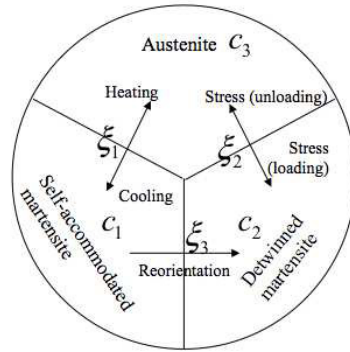


Fig 1. Internal variables for a dense SMA model [2]

SMA have had important impacts on materials used in the medical and aerospace industries [1, 2]. Release mechanisms (bolts that expand and contract) are used on airplane wings as well as recent convertible laptops/tablets (including a number of Windows 8 combinations). In space, SMAs are used in deploying solar panels, space station component joining, vehicular docking, and numerous Mars rover components. On airplanes or drones, jet engine intakes and exhausts, helicopter blade vibration control, and smart wings that will no longer have flaps, but will change shape dynamically.

The rest of the paper is ordered as follows. In Section 2 we describe a mathematical model for Joule heated SMAs. In Section 3 we describe the virtual shaker device and the DDDAS. In Section 4, we provide some conclusions and remarks on future work.

2. SMA Model

We employ a 3-D model for polycrystalline SMAs [4] that is based on a modified phase transformation diagram, which can distinguish detwinning from phase transformation behavior. The model utilizes both direct conversion of Austenite into detwinned Martensite as well as the detwinning of self accommodated Martensite. It is suitable for performing numerical simulations on SMA materials undergoing complex thermomechanical loading paths in the stress-temperature space. The model is based on thermodynamic potentials and utilizes three internal variables to predict the phase transformation and detwinning of Martensite in polycrystalline SMAs. The model has been tested extensively on complicated geometries and can deal with both complicated thermomechanical loading paths and complex geometries robustly.

In terms of temperature, we need to know in advance for a two shape device the following:

$$M_s < M_f < A_s < A_f$$

These temperatures give us ranges in temperature when the Martensite and Austenite states will start and end, respectively. In addition we need to know the stress range for shape changing.

The mass fractions of the three phases are introduced:

c_1 : self-accommodated Martensite

c_2 : detwinned Martensite

c_3 : Austenite,

where $c_1+c_2+c_3=1$, $0 \leq i \leq 3$, $i=1,2,3$. The transitions between the different species are accounted by three independent internal variables ξ_1 , ξ_2 , and ξ_3 that satisfy $c_1=c_{10}+\xi_1-\xi_3$, $c_2=c_{20}+\xi_2+\xi_3$, and $c_3=c_{30}-\xi_1-\xi_2$ (see Fig. 1).

We use a general form of the Gibbs free energy for a polycrystalline SMA that at any instance contains any of three species. Additionally, σ is the Cauchy stress and T is temperature. The equation is given by

$$G = c_1 G^{(1)}(\sigma, T) + c_2 G^{(2)}(\sigma, T) + c_3 G^{(3)}(\sigma, T) + G^{MIX}(\sigma, T, c_1, c_2, \mu^m),$$

where the $G^{(i)}$, $i=1,2,3$ are vector equations of the form

$$G^{(1)}(\sigma, T) = G^{(2)}(\sigma, T) = -\frac{1}{2\rho} \sigma : S^M : \sigma (1 - \frac{1}{\rho}) : [\alpha^M (T - T_0) + \varepsilon^m] + c [T - T_0 - T \ln(T / T_0)] - s_0^M (T - T_0) + u_0^M$$

and

$$G^{(3)}(\sigma, T) = -\frac{1}{2\rho} \sigma : S^A : \sigma (1 - \frac{1}{\rho}) : [\alpha^A (T - T_0) + \varepsilon^m] + c [T - T_0 - T \ln(T / T_0)] - s_0^A (T - T_0) + u_0^A$$

where $:$ is the double dot operator for two tensors. For a set of hardening parameters b_1^A , b_2^A , b_1^M , b_2^M , and b_{12} , the energy mixing term is given by

$$G^{MIX}(c_1, c_2) = \frac{1}{2} b_1(\dot{\varepsilon}_1) c_1^2 + \frac{1}{2} b_1(\dot{\varepsilon}_2) c_2^2 + b_{12} c_1 c_2 + \text{sgn}(\dot{\varepsilon}_1) \mu_1 c_1 + \text{sgn}(\dot{\varepsilon}_2) \mu_2 c_2, \text{ where}$$

$$\beta_i = \beta_i^A \text{ for } \dot{\varepsilon}_i > 0 \text{ and } \beta_i^M \text{ for } \dot{\varepsilon}_i < 0, \quad i = 1, 2.$$

The total inelastic strain ε^{in} is assumed to be generated only by the phase transformation and the detwinning of Martensite and is decomposed additively,

$$\varepsilon^{in} = \varepsilon^d + \varepsilon^t, \quad \varepsilon^d = \Lambda^d \dot{\xi}_3, \quad \varepsilon^t = \Lambda^t \dot{\xi}_2, \quad \Lambda^d = \sqrt{\frac{2}{3}} H \frac{dev(\sigma)}{\|dev(\sigma)\|} \text{ when } \dot{\xi}_3 > 0,$$

$$\Lambda^t = \sqrt{\frac{2}{3}} H \frac{dev(\sigma)}{\|dev(\sigma)\|} \text{ when } \dot{\xi}_2 > 0 \quad \text{and} \quad \Lambda^t = \sqrt{\frac{2}{3}} H \frac{dev(\varepsilon^t)}{\|dev(\varepsilon^t)\|} \text{ when } \dot{\xi}_2 < 0.$$

The tensors Λ^t and Λ^d specify the flow rate for the phase transformation ($A \leftrightarrow M^d$) and the detwinning of the Martensite ($M^t \rightarrow M^d$), respectively. Finally, the second law of thermodynamics is given by

$$T \dot{\eta} = -\left(\varepsilon - \varepsilon^{in} + \rho \frac{\partial G}{\partial \sigma} \right) : \dot{\sigma} - \rho \left(s + \rho \frac{\partial G}{\partial T} \right) : \dot{T} - \rho \frac{\partial G}{\partial \xi_1} \dot{\xi}_1 + \left(\sigma : \Lambda^t - \rho \frac{\partial G}{\partial \xi_2} \right) \dot{\xi}_2 + \left(\sigma : \Lambda^d - \rho \frac{\partial G}{\partial \xi_3} \right) \dot{\xi}_3 \geq 0.$$

3. DDDAS

We have concentrated on a specific, relative simple shaker device: a vibrating system consisting of a pseudoelastic NiTi SMA beam in a cantilevered-pinned configuration. This is similar to a real shaker device at Texas A&M University that we receive limited data from. A mass is clamped in the center of the beam. The entire system receives periodic vibrations over a range of frequencies in order to determine its isolation and damping capabilities (see Fig. 2) that we feed into a multiscale finite element procedure MsFEM. Our virtual device is a simpler system compared to one with porous SMA components because the SMA model can be

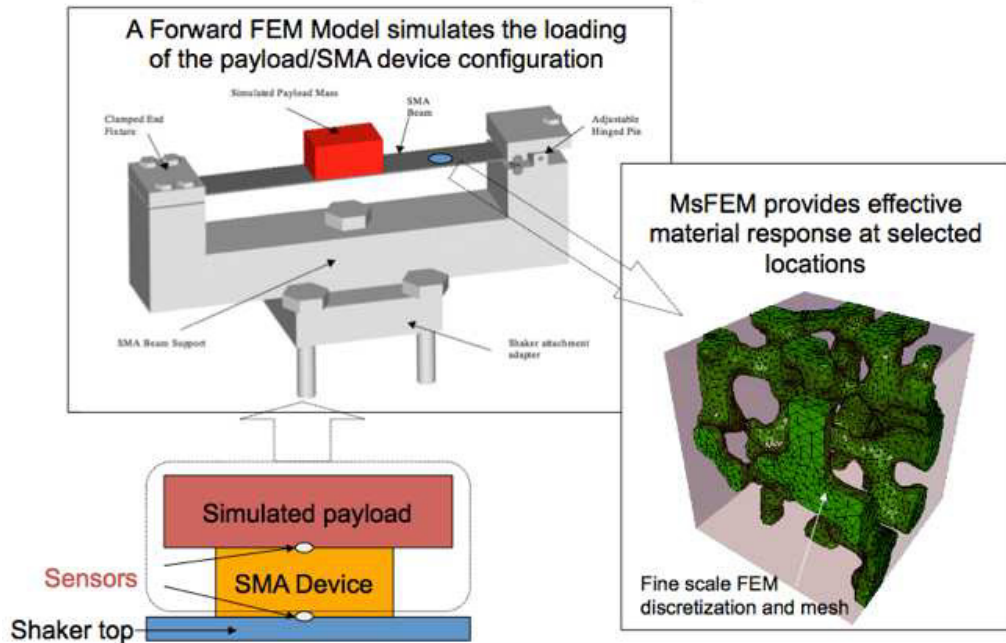


Fig. 2. Virtual shaker configuration and 3D multiscale porous SMA discretization for MsFEM code [2]

applied directly. We eliminate the homogenization step of the porous material and reduce the uncertainties in the analysis and design of the overall system.

In the virtual shaker environment we can modify the behavior of the sensors in ways that cannot be done on an existing, *very* expensive shaker table. The existing table produces data every 0.1 seconds per sensor. This may not be optimal and our DDDAS can tell each of the virtual sensors to produce data faster, slower, or temporarily stop. This capability allows us to better design future shaker tables or devices for taking payloads on aerospace vehicles.

The virtual environment allows us to vary parameters in order to study chaos, which can occur, unfortunately. Chaos is not a phenomena that is acceptable nor desired in vibration isolation devices. A careful study is required in order to guarantee that chaos is not present in such a device.

The DDDAS is realized primarily by changing the temperature of the specimen dynamically to modify its general hysteresis properties, either the Joule heating and/or the fluid flow rate in a porous SMA. Modifying the fluid pressure also lets us change the effective mechanical response.

We are able to respond to long term fatigue changes in dense SMA through model parameters. We can calibrate and improve microscale (dense) SMA model parameters based on dynamic data, e.g., the maximum transformation strain, transformation temperatures, etc. The DDDAS components interact with the forward simulations of the shaker device setup to manage data streams and feedback control.

The feedback control loop in the DDDAS is given in Fig. 3. MsFEM interacts with the DDDAS communication subsystem, which in turn communicates with the sensors. Based on the vibrations measured, we modify the SMA based on a prediction-correction process that is trained in advance, but operates dynamically.

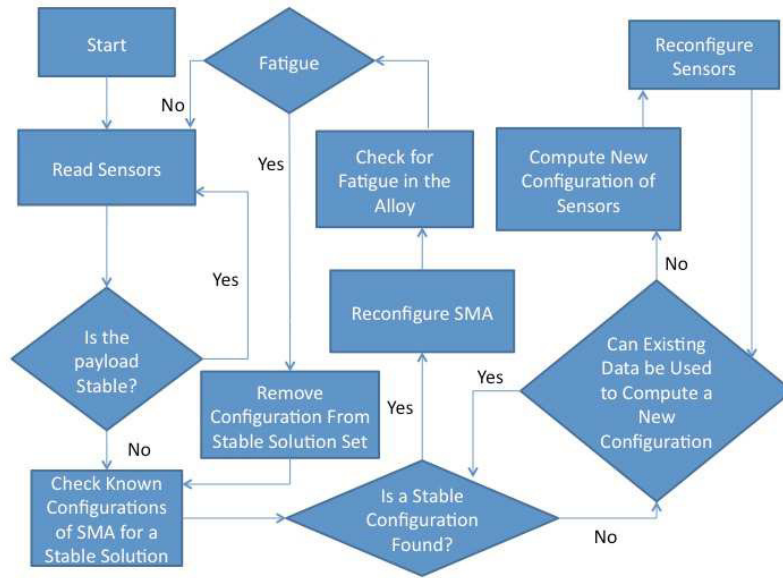


Fig. 3. DDDAS feedback control loop

Fig. 4 provides an example of a payload on the shaker table environment that goes from a steady state to a state caused by oscillation. The plot shows the (x,y) location of a single sensor at the center of the payload. Initially the sensor is at (0,0) and immediately begins moving. The sensors detect the movement and change the configuration of the SMA to stabilize the particle. The DDDAS model is used to predict the future state of the particle and the SMA is modified accordingly. Due to the chaotic nature of the vibrations the model predictions are an educated guess. Hence, sensors are required to capture the actual state of the particle and the model is updated accordingly.

Once the SMA’s shape changes the particle stabilizes and remains in a steady state until random oscillations once again require a modification in the SMA.

The oscillation used for this simulation is relatively simple oscillation that leads to two stable nodes, as seen in Fig. 4. Three dimensional oscillations have a much more complex orbit structure and can even exhibit chaos. In these cases, the need for DDDAS feedback cannot be understated.

4. Conclusions and Future Work

Progress has been made towards creating a DDDAS for a virtual shaker based on a robust model for polycrystalline Joule heated SMAs that is based on a modified phase transformation diagram and distinguishes detwinning from phase transformation behavior. We will soon be able to use historical data from a real shaker table and NiTi SMA to calibrate our virtual shaker and DDDAS. The historical data will also be used to generate more synthetic data that is realistic in order to further test, refine, and extend our DDDAS.

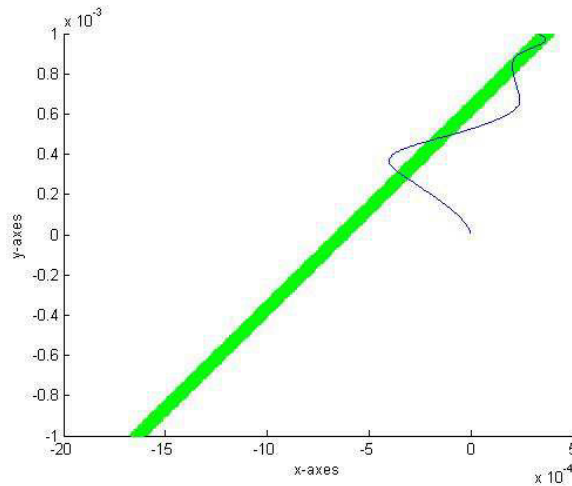


Fig. 4: Orbits of simple shaker table example

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References

- [1] Lagoudas DC, Shape Memory Alloys: Modeling and Engineering Applications, Springer, New York, 2008.
- [2] Douglas CC, Efendiev Y, Popov P, Calo V, An introduction to a porous shape memory alloy dynamic data driven application system, *Procedia Computer Science*, 9 (2012), pp. 1081-1089.
- [3] Otsuka K, Wayman CM, Shape Memory Alloys, Cambridge University Press, 1999.
- [4] Popov, P, Lagoudas DC, A 3-D constitutive model for shape memory alloys incorporating pseudoelasticity and detwinning of self-accommodated martensite, *International Journal of Plasticity*, 23 (2007), pp. 1679-1720.
- [5] Qidwai MA, Lagoudas DC, Numerical implementation of a shape memory alloy thermomechanical constitutive model using return mapping algorithms, *International Journal for Numerical Methods in Engineering*, 47 (2000), pp. 1123-1168.