ARL-TR-7872 ● Nov 2016

US Army Research Laboratory

High Performance Computing (HPC)-Enabled Computational Study on the Feasibility of using Shape Memory Alloys for Gas Turbine Blade Actuation

by Kathryn Esham, Luis Bravo, Anindya Ghoshal, Muthuvel Murugan, and Michael Walock

NOTICES

Disclaimers

ARL-TR-7872 ● NOV 2016

US Army Research Laboratory

High Performance Computing (HPC)-Enabled Computational Study on the Feasibility of using Shape Memory Alloys for Gas Turbine Blade Actuation

by Luis Bravo, Anindya Ghoshal, Muthuvel Murugan, and Michael Walock
Vehicle Technology Directorate, ARL

Kathryn Esham
Oak Ridge Institute for Science and Education (ORISE)

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE (*DD-MM-YYYY*)	2. REPORT TYPE	3. DATES COVERED (From - To)
November 2016	Technical Report	June 2016–August 2016

4. TITLE AND SUBTITLE
High Performance Computing (HPC)-Enabled Computational Study on the Feasibility of using Shape Memory Alloys for Gas Turbine Blade Actuation

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Kathryn Esham, Luis Bravo, Anindya Ghoshal, Muthuvel Murugan, and Michael Walock

5d. PROJECT NUMBER
1120-1120-99

5e. TASK NUMBER

5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
US Army Research Laboratory
ATTN: RDRL-VTP
Aberdeen Proving Ground, MD 21005-5066

8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-TR-7872

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

13. SUPPLEMENTARY NOTES

14. ABSTRACT
Creating an actuation system that can move turbine blades during flight of an aircraft requires very specific material properties. Shape memory alloys (SMAs) are an excellent option as they have a high energy density; however, they are currently lacking the high-temperature stability necessary for operation in extreme thermal conditions. To push SMAs to higher temperatures nanoprecipitates are formed, allowing the martensitic phase transformation to stabilize over many thermal cycles while increasing the transformation temperature range. How these precipitates work is not well understood, but harnessing their features aids the design of a new high-temperature SMA. This work used phase field analysis to show that the orientation of the precipitate is of special interest due to the effect on the microstructure. A precipitate oriented with the martensitic variants shows little potential for residual strain, which may lead to failure. If the precipitates are at a desired orientation, the phase transformation may be able to occur safely at much higher temperatures than previously thought.

15. SUBJECT TERMS
HPC, high performance computing, materials modeling, shape memory alloy, SMA, engines

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
					Luis Bravo
a. REPORT	b. ABSTRACT	c. THIS PAGE	SAR	24	19b. TELEPHONE NUMBER (Include area code)
Unclassified	Unclassified	Unclassified			410-278-9719

Standard Form 298 (Rev. 8/98)
Prescribed by ANSI Std. Z39.18

Contents

List of Figures

Student Biography

Impact of High Performance Computing (HPC) Internship Program Research Experience

I earned my BS in glass engineering science from Alfred State University in Alfred, New York, in May 2014. In Summer 2012, I participated in a research experience for undergraduates at Northern Illinois University in DeKalb, Illinois, where my work focused on a novel method of synthesizing boron nitride doped graphene and characterization of the material. Following this, I sought research work at Alfred University and worked with several graduate students on preparing glass samples for analysis at a national laboratory. My senior honors thesis at Alfred focused on investigating several glass compositions as possible candidates for nuclear waste storage. I joined the Anderson Group in the Materials Science and Engineering department at The Ohio State University (OSU) in January 2015 where my work is focused on computational modeling and analysis of high-temperature shape memory alloys.

Our project focused on actuating turbine blade in jet engines to improve efficiency. By actuating the blades in ascension and cruising conditions, the engine will use fuel in the most efficient manner, resulting in economic and environmental improvements for the Warfighter sponsorship.

My role in this project was to investigate the material to be used for this actuation motion. Shape memory alloys are lightweight materials with a potential for high-density power output, making them great candidates. The challenge is that they are not stable at high temperatures, but we can improve their stability by creating precipitates in the structure. HPC resources were used for computational analysis investigating various shapes and orientations of these precipitates at high temperatures. The supercomputing power allowed me to perform several simulations, which I could then compare through postprocessing. Using code developed at OSU and guidance from my mentors at Aberdeen Proving Ground (APG), Maryland, I learned more about the efficiency and power of supercomputing to analyze the shape memory alloys.

My previous research experience was all performed in an academic setting either at Alfred State, Northern Illinois, or OSU. Although I have enjoyed my time in academia, my long-term plans have always been to explore industry and working at APG this summer solidified my future career intensions.

Personally, I am used to the academic setting and way of working so the HPC internship program was a good way to step out of my comfort zone and explore how research is performed in a different environment. I found working with Dr Bravo and Dr Ghoshal to be a fun and rewarding experience because they took the time to get to know us and our individual goals, making the work environment more inclusive.

Educationally, this work complements my graduate work quite nicely. My work at OSU is focused on understanding fundamental material behaviors. At APG this summer, my thought process took this a step farther by exploring how this material can be applied to a real world problem. It was exciting to see how the basic understanding I am developing at OSU can be used in a novel way to improve the efficiency of a jet engine.

Acknowledgments

I would like to thank the following people and organizations:

- Dr Anindya Ghoshal and Dr Luis Bravo for taking me on as a summer intern and expanding my understanding of how supercomputing can be used to solve problems.
- Dr Peter Anderson at The Ohio State University (OSU) for his continuous guidance and passion for research.
- Dr Harshad Paranjape at Colorado School of Mines for his troubleshooting and explanations of the phase field code.
- The support centers for the OSU Supercomputer and the High Performance Computing (HPC) Help Desk.
- Our HPC Internship Program sponsors for their continued interest and support in our work.

INTENTIONALLY LEFT BLANK.

1. Introduction

1.1 Shape Memory Alloys (SMAs)

SMAs are a class of materials that undergo a martensitic transformation under a mechanical or thermal stress. The classic example is equiatomic nickel-titanium, commonly called nitinol or NiTi, which was developed at the Naval Ordinance Lab in 1959.[1] At temperatures exceeding 100 °C NiTi exists in the cubic austenitic structure; when cooled to room temperature the material undergoes a diffusionless transformation to a body-centered tetragonal structure. The material can be heated to the austenitic state and cooled to the martensitic state, rendering a shape change as it transforms between phases (Fig. 1).

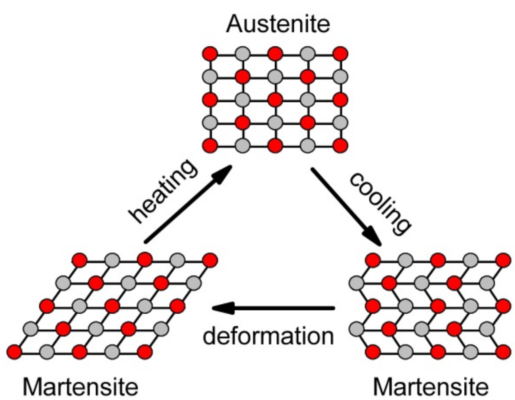

Fig. 1 Austenite to martensite transformation

In addition to the shape memory effect, this phase transformation allows for unique material properties that make SMAs attractive options for specific applications. Two such properties are superelasticity and the ability to perform mechanical work. Superelasticity or "pseudo-elasticity" refers to the ability of the SMA to recover large amounts of strain. Generally, NiTi can recover up to 6% strain without plastic deformation.[2] This allows the material to have quite a high work output. The actuation action that occurs between the austenite and martensite can be used to store mechanical energy. Together, these properties give SMAs a distinct advantage over other materials in specific applications.

There are several key temperatures that help define the phase transformation: martensitic start (M_S), martensitic finish (M_F), austenitic start (A_S), and austenitic finish (A_F). The thermal hysteresis shown in Fig. 2 illustrates the general regimes where these temperatures are defined. If the material starts in the austenitic phase and is cooled, it will begin to form when the temperature reaches M_S and continue until the M_F temperature when the material is completely transformed. At this point it can be heated and at the A_S temperature the cubic structure will nucleate and form until A_F is reached.

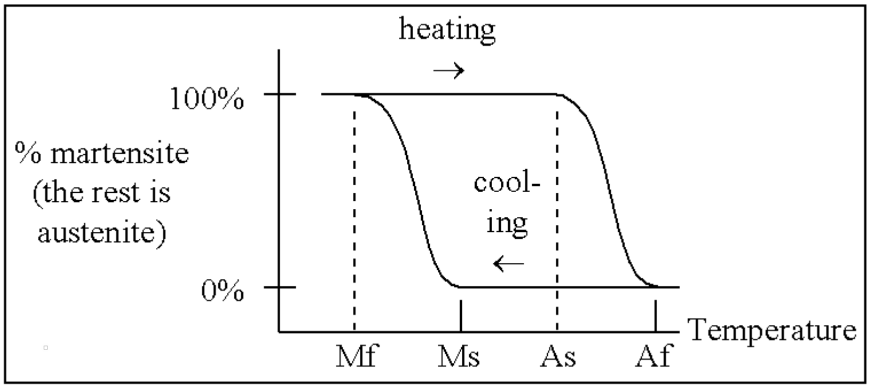

Fig. 2 Thermal hysteresis of an SMA

This thermal hysteresis defines what regime the SMA can function within. If the desired application requires a different temperature regime, the SMA needs to be tuned to match. One method of tuning SMAs involves creating nanoprecipitates in the matrix. Nanoprecipiatates provide several advantages, they suppress ratcheting during thermal cycling, reducing the possibility for failure due to creep. Additionally, they shift transformation temperatures to a higher regime and do not interfere with the transformation process.[3]

The transformation temperatures are compositionally sensitive, as demonstrated in Fig. 3. Here, the dependence of M_S is plotted as a function of nickel (Ni) content and it can be seen that as Ni shifts from 50% to 51%, M_S is reduced from approximately 75 °C to –150 °C. It would seem logical to use titanium (Ti)-rich compositions instead; however, the Ni provides stability, strength, and so forth. One way to combat this issue is to introduce precipitates by aging the material. NiTi can be aged to create Ni_4Ti_3 precipitates, which generally elevate transformation temperatures.[4] However, to push SMAs to higher temperatures a ternary system can be created. The addition of the third element results in Ni-rich precipitates that leave an Ni-depleted matrix. A matrix with an Ni deficit will have higher transformation temperatures.

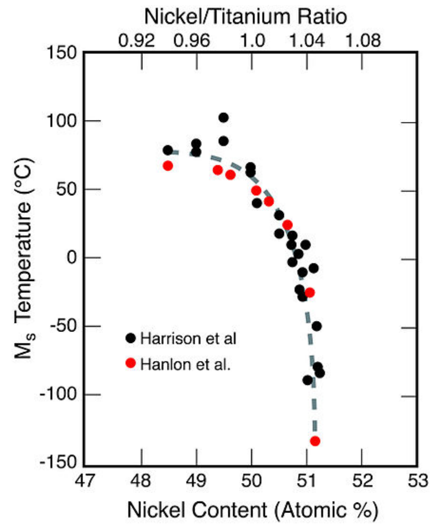

Fig. 3 Transformation temperature vs. Ni/Ti ratio

Due to the nature of the shape memory effect and superelacticity, SMAs are a unique class of materials that offer a unique solution. In the medical field, SMAs are particularly attractive due to their biocompatibility. Perhaps the best well-known application is the use of NiTi wires for medical stents.[5] The wire is tuned to the temperatures of the human body—it can be inserted in a smaller shape, and then expanded once it has reached the desired location. The constant temperature of the body ensures that the stent maintains it shape, due to a constant stress on the material. They have also been used as bone staples and porous bone implants.[6] Other common applications include orthodonture wires and eyeglass frames, where a constant stress is put to work. Although SMAs are a big player in the medical field, they also find applications in other fields such as aerospace[7] and energy.[8]

1.2 Jet Turbine Engines

Increasing the efficiency of jet turbine engines has the potential for great economic and environmental improvements. The typical jet engine consists of 5 main components: fan, compressor, combustor, turbine, and nozzle. Air is brought into the system through the fan, which directs some of the flow to the core and the rest outside to act as a coolant and noise suppressant. Air directed to the core moves to the compressor, where its volume is reduced to increase pressure and potential energy. The condensed air is then fed into the hot section of the engine starting with the combustion chamber. Here, the high-energy air is mixed with fuel and ignited; the hotter air will expand and is therefore storing more energy. As the hot air moves through the next section, the turbine blades rotate and move blades connected via a rod in the fan and compressor. Finally, the hot air exits the engine and mixes with the cold air from the initial intake, providing thrust.[9]

There are many aspects that can be modified to improve the engine's efficiency. The nozzles injecting fuel can have different shapes or hole geometry or the blade clearance throughout the engine can be modified, for example. Another promising approach involves articulating the blades in the turbine wheel.[10] Currently, there is no way to articulate the blades so the angle of pitch is one that is broadly beneficial for ascension, cursing, and dissension. If the blades could be articulated such that for each of the 3 stages they are in a different—but optimal—position, the fuel will be used more efficiently.

To introduce an actuation system into the turbine there are several material properties that need to be considered. The environment will be high temperature and pressure, and will require a high power density, long lifetime, low cost, and lightweight material. Traditional actuation systems such as hydraulic and pneumatic could provide the desired power output, but are generally too heavy and bulky to incorporate. Other material options include piezoelectric, electromotive force, or smart materials. As a subset of smart materials, SMAs are a lightweight, low-cost, and power-dense option. The challenge lies in bringing them to function in high temperatures and pressure with a reliable lifetime.

2. Methods, Assumptions, and Procedures

This work was performed using phase field analysis on the Ohio Oakley Supercomputer and Army Excalibur Supercomputer. Phase field codes are explicit, numerical solutions that replace interface boundary conditions with a partial differential equation. This phase field code uses a forth order Landau polynomial (Eq. 1) for the asymmetric transformation pathway between the austenite and martensite phases of the material. The free energy equation is calculated with elasticity, chemical and interfacial information as detailed in the (Eq. 2). This simulation reads information in a VUMAT file, which provides Abaqus with user-specified material parameters, here specific to NiTi. Additionally the simulation is provided with the slip systems allowing for the possibility of plastic deformation. Finally, the user can define the mesh used including desired size, shape, and orientation of a precipitate.

Eq. 1: Landau polynomial

$$f_{LP}(v_t,\ \theta) = \lambda\left[(\theta - \theta_{trans})\left(p\sum_{i=1}^{N_t} v_i^2 + q\left(\sum_{i=1}^{N_t} v_i^2\right)^2\right) + \left(b\sum_{i=1}^{N_t} v_i^2 + d\sum_{i=1}^{N_t} v_i^4 + f\left(\sum_{i=1}^{N_t} v_i^2\right)^2\right)\right] \tag{1}$$

Eq. 2: Free energy equation

$$\Psi_R = \frac{1}{2}\mathrm{E^eCE} + f_{LP}(v_t, \theta) + \frac{1}{2}\sum_{t=1}^{N_t} \nabla v_t \sum_{u=1}^{N_t} \mathrm{K}_{tu} \nabla v_t \quad . \tag{2}$$

The simulation in this work took advantage of the fast computational time of 2-D geometries. This representation can be derived from a 3-D model. In 3-D a cube represents the austenitic state and a brick represents the martensitic state. The brick comes from stretching the cube in x, y, or z (Fig. 4). Similarly, in 2-D austenite can be represented by a square and martensite can be represented by a rectangle, stretched in x or y. Boundary conditions include a fixed origin and rolling condition on the bottom left node. The material starts at 350 K and is immediately step-quenched to 150 K at the first time step, then held for the remaining time. This allows the transformation between austenite and martensite to be as computationally efficient as possible. Nucleation sites determine where the martensite will begin to form.

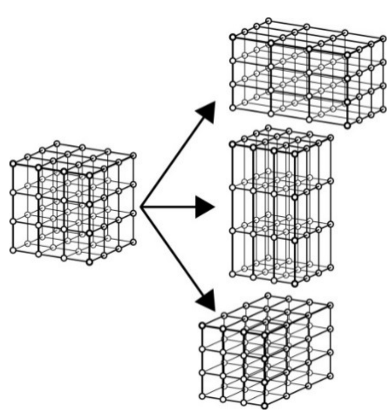

Fig. 4 3-D representation of austenite to martensite

In terms of precipitate, orientation, size and shape were values of interest to study. The goal is to look at the effect that these 3 parameters have on microstructure, transformation temperatures, and actuation properties.

The first study, detailed in this report, is a qualitative study of the effect of orientation on microstructure. An elliptical precipitate with a long axis, $a = 0.25$, short axis $b = 0.10$ (according to Eq. 3), was rotated from 0° to 45° in 15° increments. Images of the final microstructure were visualized in Abaqus CAE, version 6.14. A case without a precipitate was also run. Each case was run once.

Eq. 3: The form of an ellipse, long axis *a*, short axis *b*,

$$\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1 \quad . \tag{3}$$

Because of the output Abaqus can handle, a single variable can be plotted at a time. This means that if "Variant 1" is plotted in red, the blue is simply the absence of Variant 1 (as opposed to directly being Variant 2). Likewise, if "Variant 2" is plotted, elements identifying as Variant 2 will be red and elements not identifying as Variant 2 will be blue. For the purposes of this qualitative study, it can be assumed that red is Variant 1 and blue is Variant 2 for simplicity.

In the final step, the general structure of the martensite can be thought of as "compatible" or "incompatible". Here the difference between compatible and incompatible is the alignment of the precipitate and martensite plates. If there is a good alignment, stress will be reduced locally creating a compatible situation. If there is not a good alignment—which could lead to plates stretching or shrinking to accommodate—the precipitate will experience a local stress, in an incompatible situation. The benefits or detriments of stress will be addressed later, but are helpful for distinguishing the difference between compatible and incompatible.

3. Results and Discussion

The initial study investigated the distribution of martensite around the precipitate as a function of orientation. As previously detailed, the precipitate has a long axis and a short axis. The patterns formed relative to each axis are discussed with regard to the "interruption" of one variant by the other.

In the case with no precipitate, the final step shows the plot of Variant 1 in red. The blue areas are assumed to be Variant 2. In this case the 2 variants form an alternating striated pattern, which is expected as the material experiences twinning in the martensite. Generally, the pattern is continuous (Fig. 5).

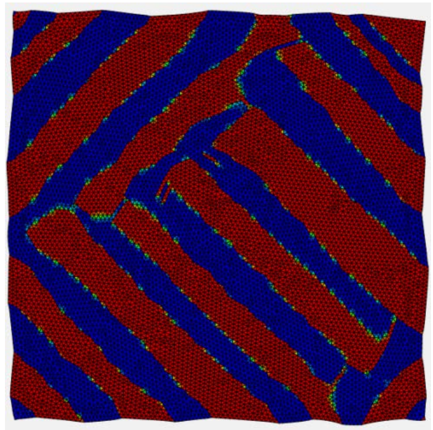

Fig. 5 Phase field simulation without a precipitate

Now we add in the precipitate at 0°, the material is cooled and the striated pattern form again. This time, there appears to be some disruption in the line orthogonal to the long axis of the precipitate. Here, variants span approximately half the length expected, only to be interrupted by the alternate variant type. Although the interrupted striations are most notable in this direction, there is interruption in the direction orthogonal to the short axis as well (Fig. 6).

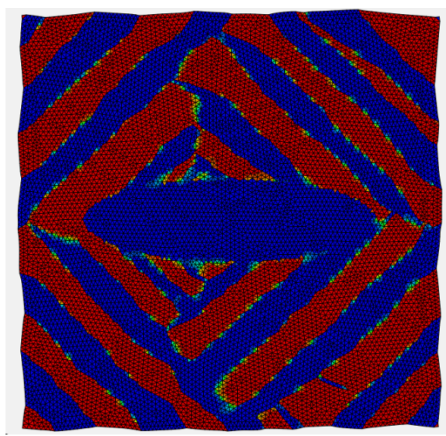

Fig. 6 Phase field simulation with precipitate oriented at 0° to the horizontal axis

Next, the precipitate is rotated to 15°. Here, the interrupted variants have a much smaller width, particularly closer to the precipitate. It seems as though the interruption does not extend as far through the material as in the 0° case, but remains more local (Fig. 7).

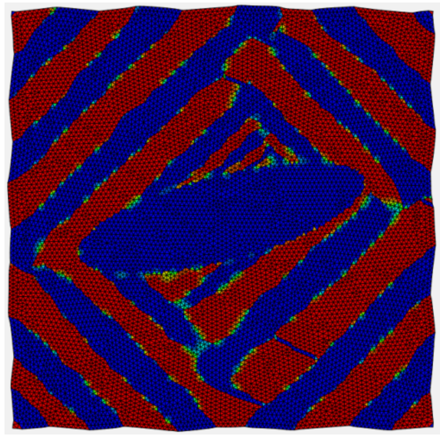

Fig. 7 Phase field simulation with precipitate oriented at 15° to the horizontal axis

As the precipitate is moved to the 30° position, the interruption in martensite variants in the direction parallel to the long axis has almost completely disappeared. Small interruptions exist very locally around the ends of the precipitate, where the plates are again smaller than the 0° case (Fig. 8).

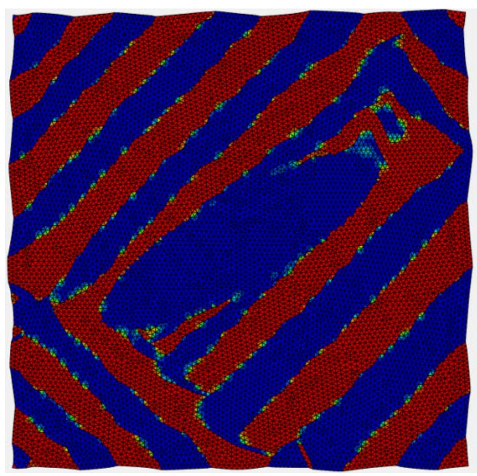

Fig. 8 Phase field simulation with precipitate oriented at 30° to the horizontal axis

Finally, the precipitate is rotated to 45° where it appears to be aligned with the martensite plates that form. Although there appears to be little interruption on the long axis, there is minor interruption parallel to the short axis on a very local scale. Overall, the interruption does not extend past 2 plates, keeping it relatively local (Fig. 9).

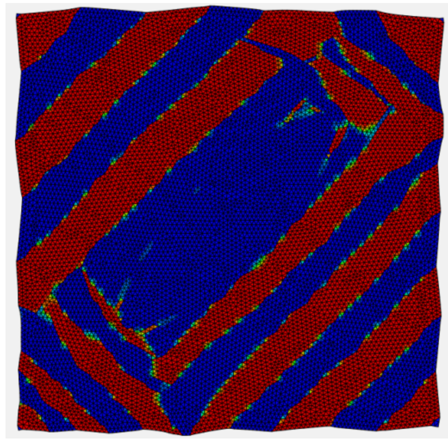

Fig. 9 Phase field simulation with precipitate oriented at 45° to the horizontal axis

The interruption is of interest because the existence of an interface makes stress concentration development or residual strain more likely. If the edge of the precipitate is in an incompatible alignment with the variant pattern in the matrix, there is likely stress at the interface between precipitate and matrix. Although plastic deformation in the form of residual strain is not desirable, the ability to control what type of variant forms where is desirable. If the local stress concentrations around the precipitate can dictate which type of variant forms, it can select for the more compatible variant during the next thermal cycle. This essentially allows the precipitate to become a nucleation site. A controlled microstructure means a more stable material and in turn a reliable, long-lasting option for high-temperature actuation applications.

4. Conclusions

Creating an actuation system that can move turbine blades during flight of an aircraft requires very specific material properties. SMAs are an excellent option as they have a high energy density; however, they are currently lacking the high-temperature stability necessary for operation in extreme thermal conditions. To push SMAs to higher temperatures nanoprecipitates are formed, allowing the martensitic phase transformation to stabilize over many thermal cycles while increasing the transformation temperature range. How these precipitates work is not well understood, but harnessing their features aids the design of a new high-temperature SMA. This work used phase field analysis to show that the orientation of the precipitate is of special interest due to the effect on the microstructure. A precipitate oriented with the martensitic variants shows little potential for residual strain, which may lead to failure. If the precipitates are at a desired orientation, the phase transformation may be able to occur safely at much higher temperatures than previously thought.

5. Recommendations and Future Work

Before SMAs can be implemented into high-temperature actuation systems, they need cyclic stability. Through the use of this phase field analysis, the local stress around a precipitate can be used to create a stable material. Quantitatively, there is still much work to do in determining local stresses. Once the optimal precipitate's size, shape, and orientation have been selected due to their effect on the microstructure, transformation temperatures, and actuation properties through this phase field analysis; then the information can be fed into a larger scale model. Due to the application of creating an SMA for turbine blade actuation, predictions beyond the scale of phase field calculations is necessary. Microstructural finite-element simulations perform calculations on a larger scale. This model can be informed by the phase field output as well as data collected from experimental work done at National Aeronautics and Space Administration's Glenn Research Center and The Ohio State University. Together this information will provide a material that can perform work at high temperatures, which can be fed into the microstructural simulation that will speak to the feasibility of implementing SMAs as actuators in jet turbine engines.

6. References

1. Nickel titanium. Wikimedia Foundation Inc.; 2016 Oct 4 [accessed 2016 Aug 25]. https://en.wikipedia.org/wiki/Nickel_titanium.
2. Nemat-Nasser S, Wei-Guo G. Superelastic and cyclic response of NiTi SMA at various strain rates and temperatures. Mechanics of Materials. 2006;38.5-6:463–74.
3. Anderson P. Fundamentals and applications of ambient and high-t shape memory alloys. Thermal Actuation: Effect of Aging. 2015.
4. Khalil-Allafi J, Antonin D, Gunther E. Ni4Ti3-precipitation during aging of NiTi shape memory alloys and its influence on martensitic phase transformations. Acta Materialia. 2002;50.17:4255–274.
5. Duerig T, Pelton A, Stöckel D. An overview of nitinol medical applications. Materials Science and Engineering: A. 1999;149-60:273–275.
6. Bansiddhi A, Sargeant TD, Stupp SI, Dunand DC. Porous NiTi for bone implants: a review. Acta Biomaterialia 2008;4.4:773–82.
7. Mabe JH, Ruggeri RT, Rosenzweig E, Yu C.-JM. NiTinol performance characterization and rotary actuator design. p. 95–109. Vol. 5388.
8. Menna C, Auricchio F, Asprone D. Chapter 13, Applications of shape memory alloys in structural engineering. In: Concilio LL, editor. Shape Memory Alloy Engineering. Boston (MA): Butterworth-Heinemann; 2015. p. 369–403.
9. Shaw RJ. Engines: how does a jet engine work? Engines. NASA Glenn Research Center, n.d. 2016 Aug 25.
10. Murugan M, Booth D, Ghoshal A, Thurman D, Kerner K. Concept study for adaptive gas turbine rotor blade. The International Journal of Engineering and Science. 2015;4.9:10–17.

List of Symbols, Abbreviations, and Acronyms

2-D	2-dimensional
3-D	3-dimensional
A_F	austenitic finish
A_S	austenitic start
APG	Aberdeen Proving Ground
HPC	high performance computing
M_F	martensitic finish
M_S	martensitic start
Ni	nickel
OSU	The Ohio State University
SMA	shape memory alloy
Ti	titanium

1 (PDF)	DEFENSE TECHNICAL INFORMATION CTR DTIC OCA
2 (PDF)	DIRECTOR US ARMY RESEARCH LAB RDRL CIO L IMAL HRA MAIL & RECORDS MGMT
1 (PDF)	GOVT PRINTG OFC A MALHOTRA
6 (PDF)	DIR USARL RDRL VT E RIGAS W WINNER RDRL VTP L BRAVO A GHOSHAL M MURUGAN M WALOCK

INTENTIONALLY LEFT BLANK.