Phase Field Modeling of Martensitic Phase Transformation in Nitinol

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Introduction

Nitinol (NiTi), is a Shape Memory Alloy (SMA) composed of nickel (Ni) and titanium (Ti). SMAs are characterized by the Shape Memory Effect (SME), which results from a crystalline phase change known as “Thermoelastic Martensitic Transformation”. If the material is deformed and then heated, Nitinol’s crystallographic arrangement changes from monoclinic (Martensite) to cubic (Austenite), recovering its original pre-deformed microstructure. These characteristics makes Nitinol useful for many biomedical and industrial applications.

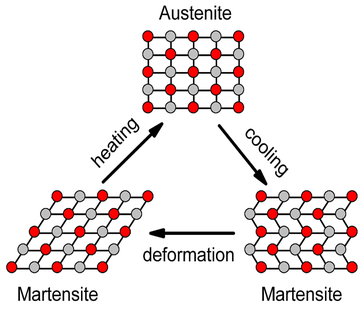

Figure 1: Martensitic Phase Transformation (MPT)

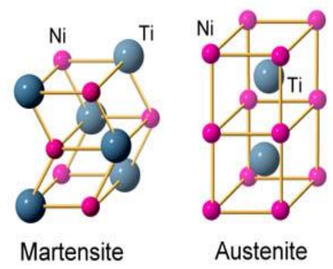

Figure 2: Crystallographic Arrangements of NiTi

Objectives

Develop a 2D phase field model to study the Martensitic Phase Transformation in NiTi

Establish a phase field methodology that is generally applicable to distinct SMAs

Conduct simulations in a temperature regime in which the alloy exhibits the SME

Methods

Figure 3: Methodology for MPT Simulation

The total Gibbs free energy for a proper MPT is defined as the sum of the local and elastic free energy densities and the coupling of the transformation strain tensor ε_t through a 2-3-4 polynomial $\varphi(\eta)$, where a is a constant and η is the order parameter.

$$F_{Gibbs} = F_{loc} + F_{el} + \varepsilon_t \varphi(\eta)$$

$$\varphi(\eta) = a\eta^2 + (4-2a)\eta^3 + (a-3)\eta^4$$

$$0 \le a \le 6\,;\; 0 \le \eta \le 1$$

F_{loc} is expressed as a 2-3-4 polynomial, dependent on the temperature T and η.

$$F_{loc} = F(T,\eta) = A\eta^2 + (4\Delta G^T - 2A)\eta^3 + (A - 3\Delta G^T)\eta^4$$

A is constant and ΔG^T is the change is Gibbs free energy from Austenite to Martensite. For the simulation, the temperature was reduced from 333K to 100K to generate a temperature-induced MPT. For $a = 3$ and theΔT described above, $F(T,\eta)$ and $\varphi(\eta)$ are defined as:

$$\varphi(\eta) = 3\eta^2 - 2\eta^3$$

$$F(T,\eta) = -1021\eta^2 + 470\eta^3 + 158\eta^4$$

Results

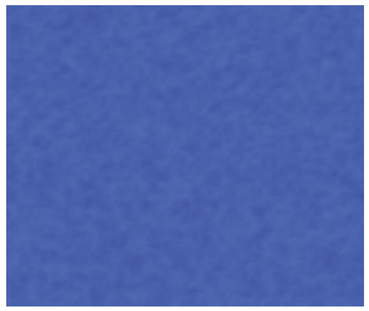

Figure 4: Initial Microstructure

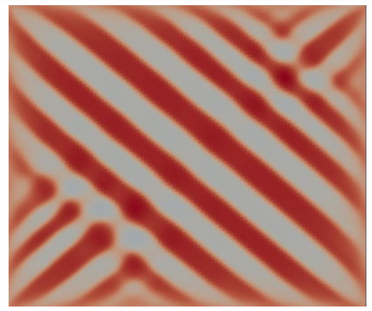

Figure 5: Final Microstructure

Austenite **Martensite Var. 1** **Martensite Var. 2**

The mesh grids are colored by the value of the order parameter η, representing different microstructure variants. The simulation conducted utilized a reference code that is being refined. Similar results are hypothesized.

Conclusion

- The Ginzburg-Landau theory is a practical approach to understand the relationship between the Austenite and Martensite phases
- Different temperature-induced Martensite variants may coexist within the material as a result of distinct twinned microstructure arrangements

Future Work

Revise the MOOSE input parameters for quantitative modeling of MPT in NiTi

Apply the described phase field model to distinct SMAs to study their microstructure evolution

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