The unique ability of shape memory alloys (SMAs) to remember and recover their original shape after large deformation offers vast potential for their integration in advanced engineering applications. SMAs can generate recoverable shape changes of several percent strain even when opposed by large stresses owing to reversible deformation mechanisms such as twinning and stress-induced martensite. For the most part, these alloys have been largely used in the biomedical industry but with limited application in other fields. This limitation arises from the complexities of prevailing microstructural mechanisms that lead to dimensional instabilities during repeated thermomechanical cycling. Most of these mechanisms are still not fully understood, and for the most part unexplored. The objective of this work was to investigate these deformation and transformation mechanisms that operate within the low temperature martensite and high temperature austenite phases, and changes between these two states during thermomechanical cycling. This was accomplished by combined experimental and modeling efforts aided by an in situ neutron diffraction technique at stress and temperature.

The primary focus was to investigate the thermomechanical response of a polycrystalline Ni49.9Ti50.1 (in at.%) shape memory alloy under uniaxial deformation conditions. Starting with the deformation of the cubic austenitic phase, the microstructural mechanisms responsible for the macroscopic inelastic strains during isothermal loading were investigated over a broad range of conditions. Stress-induced martensite, retained martensite, deformation twinning and slip processes were observed which helped in constructing a deformation map that contained the limits over which each of the identified mechanisms was dominant. Deformation of the monoclinic martensitic phase was also investigated where the microstructural changes (texture, lattice strains, and phase fractions) during room-temperature deformation and subsequent thermal cycling were captured and compared to the bulk macroscopic response of the alloy. This isothermal deformation was found to be a quick and efficient method for creating a strong and stable two-way shape memory effect.

The evolution of inelastic strains with thermomechanical cycling of the same NiTi alloy, as it relates to the alloy stability, was also studied. The role of pre-loading the material in the austenite phase versus the martensite phase as a function of the active deformation modes (deformation processes as revealed in this work) were investigated from a macroscopic and microstructural perspective. The unique contribution from this work was the optimization of the transformation properties (e.g., actuation strain) as a function of deformation levels and pre-loading temperatures. Finally, the process used to set actuators, referred to as shape setting, was investigated while examining the bulk polycrystalline NiTi and the microstructure simultaneously through in situ neutron diffraction technique at stress and temperature.

Knowledge gained from the binary NiTi study was extended to the investigation of a ternary Ni-rich Ni50.3Ti29.7Hf20 (in at.%) for use in high-temperature, high-force actuator applications. This alloy exhibited excellent dimensional stability and high work output that were attributed to a coherent, nanometer size precipitate phase that resulted from an aging treatment.

Finally, work was initiated as part of this dissertation to develop sample environment equipment with multiaxial capabilities at elevated temperatures for the in situ neutron diffraction measurements of shape memory alloys on the VULCAN Diffractometer at Oak Ridge National Laboratory. The developed capability will immediately aid in making rapid multiaxial measurements on shape memory alloys wherein the texture, strain and phase fraction evolution are followed with changes in temperature and stress.

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The public is welcome to attend.