Polycrystalline NiTi shape memory alloys have the ability to recover their original shape against external loads when heated through a phase transformation from a lower-symmetry B19’ martensite phase to a higher-symmetry B2 austenite phase. The strain associated with a shape memory alloy in an actuator application typically has thermal, elastic and inelastic contributions. The objective of this work was to investigate the aforementioned strains by recourse to in situ neutron diffraction experiments during selected combination of heating, cooling and/or mechanical loading. The studies were conducted on polycrystalline Ni49.9Ti50.1 specimens on the Spectrometer for Materials Research at Temperature and Stress at Los Alamos National Laboratory.

First, the lattice strain evolution during heating and cooling in an unloaded sample was studied. The lattice strain evolution remained linear with temperature and was not influenced by intergranular stresses, enabling the determination of a thermal expansion tensor that quantified the associated anisotropy due to the symmetry of B19’ NiTi. The tensor thus determined was subsequently used to obtain an average coefficient of thermal expansion that was consistent with macroscopic dilatometric measurements and a 30,000 grain polycrystalline self-consistent model.

Second, the elastic response of B19’ martensitic NiTi variants during monotonic loading was studied. Emphasis was placed on capturing and quantifying the strain anisotropy which arises from the symmetry of monoclinic martensite and internal stresses resulting from intergranular constraints between individual variants and load re-distribution among variants as the texture evolved during detwinning and variant reorientation processes. Plane specific elastic moduli were determined from neutron measurements and compared with those determined using a self-consistent polycrystalline deformation model and from recently reported elastic stiffness constants using an ab initio approach. The comparison among the three approaches further helped understand the influence of elastic anisotropy, intergranular constraint, and texture evolution on the deformation behavior of polycrystalline B19’ NiTi.

Lastly, the role of upper-cycle temperature, i.e., the maximum temperature reached during thermal cycling, was investigated during load-biased thermal cycling of NiTi shape memory alloys at selected combinations of stress and temperature. Results showed that the upper-cycle temperature under isobaric conditions significantly affected the amount of transformation strain. The changes in transformation strain were closely related to the evolution in texture of the room temperature martensite as well as phase volume fraction of the retained martensite in the austenite state. Additionally, multiple thermal cycles were performed under load-biased conditions in both NiTi and NiTiPd alloys, to further assess and understand the role of retained martensite. Dimensional and thermal stabilities of these alloys were correlated with the volume fraction and texture of retained martensite, and the internal strain evolution in these alloys.

This work not only established a methodology to study the thermal and elastic properties of the low symmetry B19’ monoclinic martensite, but also provided valuable insight into quantitative micromechanical and microstructural changes responsible for the thermomechanical response of NiTi shape memory alloys. It has immediate implications for optimizing shape memory behavior in the alloys investigated, with extension to high temperature shape memory alloys with ternary and quaternary elemental additions, such as Pd, Pt and Hf.

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