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Neutron diffraction studies and multivariant simulations of shape memory alloys: Empirical texture development–mechanical response relations of martensitic nickel–titanium

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Abstract

Mechanical responses and texture developments were observed in situ during the creation of multiaxial stress states in polycrystalline NiTi parallelepiped specimens, achieved via sequential compression along unique principal axes. For all of the compression stages, regardless of initial texture, the two major texture components behaved similarly: (1 0 0) poles aligned with, while (0 1 1) poles oriented perpendicular to, the loading direction. The effective critical resolved shear stress needed to induce significant reorientation, however, was reduced through prior loading. In the macroscopic responses, prior transverse direction loading resulted in widening of the reorientation plateau, a reduction of the effective Young's modulus, and substantial alteration of effective Poisson's ratios during axial direction straining. Additionally, these empirical results are presented in a manner conducive to the verification of shape memory alloy micromechanics and continuum mechanics constitutive models.

Keywords: Shape memory alloys (SMA); Compression test; Texture; Neutron diffraction; Twinning

1. Introduction

Shape memory alloys (SMAs), one of a class of smart or active materials, can recover large strains when heated above their transformation temperatures (shape memory effect) or upon load removal (superelasticity) due to reversible solid-state phase transformation and crystallographic reorientation. In addition to shape memory behaviors, other characteristics of the phase transformation, such as hysteresis, latent heat release and change in electrical resistance, enable SMAs to have a variety of applications in numerous industries, including medical, aerospace, defense, consumer technology, automotive and telecommunications. Among many alloy systems exhibiting shape memory behaviors, nickel–titanium (NiTi, Nitinol) is the most prevalent in commercial applications due to its large recoverable strain, superior fatigue performance and biocompatibility.

Nitinol is commercially available in various forms: bar, tube, rod, wire, sheet, ribbon and thin film. In all of these conditions, even in one- and two-dimensional forms such as wire or thin film, crystallographic texture development plays a very important role and can lead to drastic changes in the alloy's thermomechanical responses. Through calculation, it has been shown that recoverable deflection sensitivity to film texture differs between major alloy systems [1], agreeing with the work in Refs. [2–4]. Thin NiTi plates have also been fabricated via cold rolling, and dependence of deformation or recrystallization texture on annealing

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temperature and rolling reduction were found in addition to directional dependence of transformation [3]. Related studies on rolled sheets have shown similar results [5–9]. More recently, digital imaging correlation has been used to examine these relationships [10]. In addition to examining films, plates and sheets, relationships between microstructure and the tensile responses of NiTi wires have been reported [11], as well as texture-dependent effects in other NiTi forms: tension–compression asymmetry in both single crystals and polycrystalline rods [12], cyclic behaviors of rectangular single-crystal specimens [13], and fatigue properties of hot-rolled and cold-drawn rods [14].

Among the previous work, the experimental research focused mostly on measuring austenite texture at various points in the processing paths while observing transformation strain, and in several of the studies, pre-load martensite texture and subsequent stress–strain responses were also characterized [11–14]. Utilizing Spectrometer for MAterials Research at Temperature and Stress (SMARTS) [15] at Los Alamos Neutron Science Center (LANSCE), the evolution of internal elastic strains, crystallographic orientation, volume fraction, coefficient of thermal expansion, and strain during in situ thermomechanical loading of bulk NiTi systems has been monitored [16–20]. However, due to the configuration of SMARTS, the study of the texture evolution was limited to two specimen orientations (i.e. diffraction vectors along perpendicular and parallel sample directions), hence complete orientation distribution functions (ODFs) could not be obtained from the collected data.

In the current study, in addition to recording pole peak intensity evolutions along an axial and transverse specimen direction in situ using SMARTS, complete ODFs of the 54.8 wt.% NiTi specimens were measured ex situ via neutron diffraction using HIgh Pressure Preferred Orientation diffractometer (HIPPO) [21] at critical points of the loading sequences. Broadly speaking, these experiments were designed to meet four primary objectives:

(1) to explore the effects of loading along either a transverse or axial direction of a parallelepiped specimen;
(2) to allow for comparison of behaviors of specimens with unique initial textures subjected to the same loading condition;
(3) to observe the creation of multiaxial stress states such that the macro- and microscale behaviors associated with such a process may be correlated;
(4) to collect the data in such a manner that their presentation not only furthers fundamental understanding of the material, but also facilitates verification of SMA constitutive models.

Discussion of the data as they pertain to these objectives follows in this paper, exploring the empirically observed ties between crystallographic orientations and mechanical behaviors. In concurrent work, the final objective is realized as these data are used to verify the simultaneous mechanical response and texture development predictions of a mainstream, multivariant, micromechanics model for the first time [22], namely the simplified multivariant model [23]. Previously, to the best of the authors' knowledge, only virgin austenite texture measurements had been empirically and numerically compared for the purpose of model calibration. To make these data applicable not only to micromechanical models, but also to phenomenological constitutive models, the in situ deformation processes were repeated ex situ such that the crystallographic data are complemented by triaxial macroscopic flow curves and effective Poisson's ratios, results that would not have been possible via neutron diffraction measurements alone.

2. Experimental details

2.1. Specimen preparation

A cast cylindrical ingot of 54.8 wt.% NiTi was purchased from Special Metals (now SAES Smart Materials, New Hartford, NY). Parallelepiped specimens 8 mm × 8 mm × 20 mm were electrical discharge machined such that their axial direction (1-direction as defined in Fig. 1) coincided with the cylindrical axis of the ingot. Specimens in this state, prior to any loads being applied, are hence referred to as "virgin" specimens. The stress-free transformation temperatures of this composition have been reported as $M_f \approx 316$ K and $A_f \approx 363$ K [24], though they are not critical in the ensuing discussion except to note that the material was fully martensitic at room temperature.

2.2. Neutron diffraction measurements

In situ neutron diffraction measurements were performed using the SMARTS instrument at the Manuel Lujan Jr. Neutron Scattering Center of Los Alamos National Laboratories. SMARTS has been discussed elsewhere [15] and only a brief description will be given here. Fig. 2 shows a schematic of the specimen and the diffraction configuration with the diffraction plane in the plane of the paper (in-plane or top view). SMARTS accepts a pulsed white beam of neutrons generated through spallation reactions in a tungsten target and moderated by a water moderator at 283 K. The incident neutron beam impinges on a specimen and is scattered in all directions. Two detector banks consisting of 196 He-filled tubes are

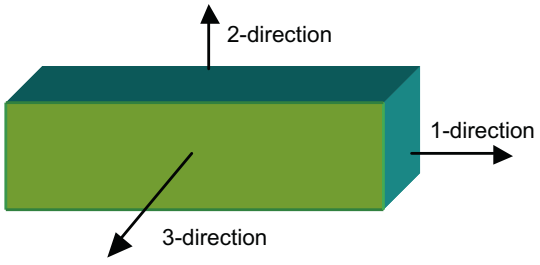

Fig. 1. Oblique view of the specimen and its coordinates.