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Competing accommodation mechanisms of the martensite in nanocrystalline NiTi shape memory alloys

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Abstract

Two competing mechanisms that compensate the transformation strains of the martensite are observed by transmission electron microscopy studies of nanocrystalline NiTi alloys. A single variant of compound twinned martensite forms below a critical grain size of about 100 nm. In larger grains, a herringbone morphology of two different twinned variants of the martensite is observed. Calculations show that homogeneous transformation strains are reduced by the self-accommodating arrangement of different martensitic variants. This takes place at the expense of the formation of additional interfaces causing local strain concentrations. It is concluded that the size dependence of the martensitic morphology is caused by a different scaling behavior of the homogeneous and interfacial strain energies.

Keywords: NiTi; Nanocrystalline; Size effects; Twinning; Self-accommodation

1. Introduction

Martensitic phase transformations are characterized by the formation of symmetry related variants of the martensite building complex microstructures on different length scales [1]. The shape strains that occur during the transformation from the parent austenitic phase to the martensite of lower crystalline symmetry force arrangements of fine mixtures of compensating variants that minimize the free energy [2]. By this process, the twinned martensitic microstructure strongly depends on the crystallography of the transformation. Similar, a small grain size of the parent phase can impose geometrical constraints that might significantly affect the martensitic morphology [3] and even the stability range of the martensite [4].

Unique thermomechanical characteristics of the shape memory effect and superelasticity can arise by a martensitic phase transformation that strongly depend on the morphology of the martensite. NiTi alloys are the most important practically used shape memory alloys [5]. Surpassing their conventional coarse-grained counterparts, bulk nanocrystalline NiTi alloys attract considerable interest as advanced functional materials [6]. In nanograins of NiTi, a unique transformation path that leads to the formation of twins at a nanometer scale is encountered [4,7]. Self-accommodation of the martensite can occur by a herringbone pattern of twinned martensitic variants separated by invariant junction planes [8]. It is the aim of the present study to investigate the dependence of the martensitic morphology on the grain size of nanocrystalline NiTi alloys using transmission electron microscopy (TEM) methods and calculations of the transformation energy.

2. Experimental procedure

A NiTi alloy with a nominal chemical composition of 50.3 at.% Ti was annealed at 800 °C; upon cooling to room temperature (RT), the martensitic phase transformation from the cubic B2 structure to the monoclinic B19′ martensite occurs that is complete at RT. The martensitic alloys were subjected to severe plastic deformation by high pressure torsion (10 turns at 6 GPa) leading to amorphization. Nanocrystallization was obtained by the polymorphous devitrification of the intermediate amorphous phase; to achieve complete crystallization and grain sizes in the range from 5 to 350 nm, specimens were annealed at different temperatures from 350 to 450 °C for 0.5 to 5 h. To achieve the martensitic phase transformation in the nanograins,

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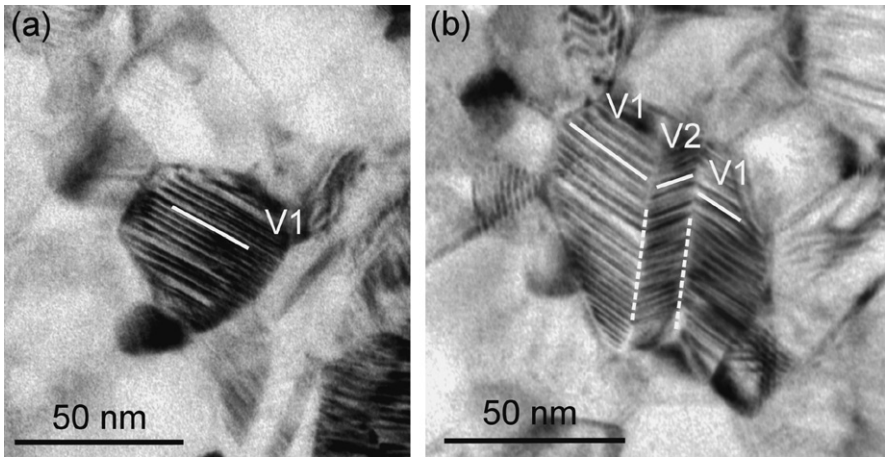

Fig. 1. TEM images of martensitic nanograins in NiTi. Atomic scale compound twins of B19′ are parallel to the full lines. (a) Single variant of twinned martensite. (b) Herringbone morphology of two variants V1 and V2 of twinned martensite (dashed lines indicate the junction planes of V1 and V2).

the specimens were quenched into liquid nitrogen. Specimens for transmission electron microscopy were prepared by twin jet polishing (for details see [4,8]). The martensitic microstructures were analyzed at RT using a CM20 operating at 200 kV and a Philips CM30 ST (operating at 250 and 300 kV) equipped with a slow scan CCD camera.

3. Experimental results

Most of the nanograins analyzed by TEM have a polygonal shape and are separated from each other by sharp grain boundaries. The nanograins do not contain dislocations and show only little lattice strains. In nanograins of a size <50 nm, martensite was not observed. Fig. 1a and b shows TEM bright-field images of grains of different size (diameter of about 50 and 100 nm, respectively) that contain B19′ martensite. In the TEM bright-field images, twins of the martensite lead to fine striations. The twins form at a nanometer scale and cause an ultrahigh density of the twin boundaries. A crystallographic analysis of the twins was carried out by high-resolution transmission electron microscopy and selected area diffraction yielding the result that the twins are of the (0 0 1) compound type. The twins have equal volume fractions and their average width is about 2 nm. Different martensitic morphologies are observed in grains of different size: in grains <100 nm, frequently a single variant of twinned martensite is encountered (cf. Fig. 1a). In grains >100 nm, a banded structure of two alternating variants V1 and V2 of the twinned martensite occurs (cf. Fig. 1b). The angle between the (0 0 1) twin boundary planes (cf. the full lines) is 125°. Additional interfaces arise between the variants V1 and V2 that are indicated by dashed lines. The width of the variant V2 is about 22% of the grain size (measured in a direction normal to the dashed lines).

4. Finite element method calculations

For the modeling of the twinned martensitic nanostructures, calculations by means of the finite element method were carried out. Using a two-dimensional approach allows to set up a parametric study within a reasonable computing time. Martensitic nanograins (cf. Fig. 1) were modeled as disc shaped inclusions contained in an elastic continuum of retained austenite (cf. Fig. 2). The complex strains $\boldsymbol{\varepsilon}$ and stresses $\boldsymbol{\sigma}$ caused by the twinned variants of the martensite were calculated considering inclusions that are made up of two different lamellae each containing a band shaped sequence of twins. Their piecewise affine deformations correspond to alternating sequences of the eigenstrains $\boldsymbol{\varepsilon}_{\mathrm{T}}^{(k)}$ and $\boldsymbol{\varepsilon}_{\mathrm{T}}^{(k')}$. In the present case, a small strain setting of the transformation strains $\boldsymbol{\varepsilon}_{\mathrm{T}}^{(k)}$ ($k = 1, 1', 2, 2', \ldots, 6, 6'$) of the 12 monoclinic Bain correspondence variants (BCVs) was used. The compound twinned variants V of the martensite are composed of BCVs that have the same index k with and without a prime (using the notation outlined by [8,9]). Different BCVs are shown by different shades of gray in Fig. 2. Corresponding to the experimental result (cf. Fig. 1b), the components of the $\boldsymbol{\varepsilon}_{\mathrm{T}}^{(k)}$ of BCV1 and BVC1′ (forming the compound twinned variant V1) and BCV3 and BCV3′ (variant V2) were calculated in a $[1\,1\,\bar{1}]_{\mathrm{B2}}$ projection. Both the twin boundaries and the junction planes are perpendicular to $[1\,1\,\bar{1}]_{\mathrm{B2}}$ and appear as lines in the sketch of

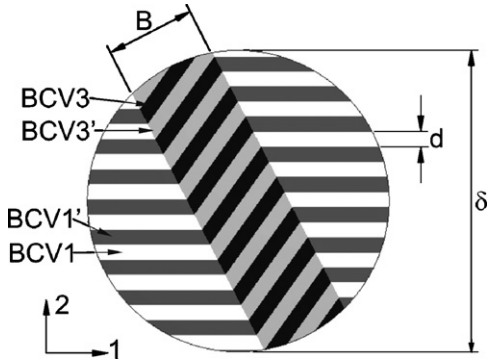

Fig. 2. Herringbone pattern of twinned variants of B19′ martensite. Each variant is composed of two Bain correspondence variants that show a compound twin relationship with respect to each other. The grain size (δ), the twin width (d) and the width of the central twinned variant B are indicated.