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An explanation of phase deformation tension–compression asymmetry of TiNi by means of microstructural modeling

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ABSTRACT

Phase deformation of mono- and polycrystalline TiNi specimens due to the direct martensitic transformation is simulated by means of a microstructural model. These simulations show that the deformation of a polycrystalline specimen loaded by a constant stress and cooled down across the temperature interval of the direct martensitic transformation depends on the mode of the stress being much less in the case of compression than in the case of tension. For most orientations of a single crystal modeling predicts a positive tension–compression asymmetry: the phase deformation in tension dominates over that in compression. Only for few orientations a small negative asymmetry is observed. A hypothesis is suggested that the positive tension–compression asymmetry of the phase deformation is inherent to TiNi because of the specific value of the third invariant of the Bain's deformation tensor. This hypothesis explaining the experimentally observed tension–compression asymmetry of untextured TiNi polycrystals is supported by microstructural modeling. Modeling also shows how the texture when it exists affects the phase deformation. By varying only the third invariant of the Bain's deformation tensor one can construct a model material either having no tension–compression asymmetry or having a negative asymmetry when the strain in tension is less than that in compression.

1. Introduction

A well-known experimental fact is that stress–strain curves of TiNi-based shape memory alloys (SMAs) loaded in tension and in compression are different [1–4], in other words, these alloys demonstrate a tension–compression asymmetry. It is natural that the reasons of this phenomenon shall be specific geometrical characteristics of the martensitic transformation. The authors of works [1,2] observed that the asymmetry is positive (deformation occurs at a significantly less stress in tension than in compression) for polycrystals and for single crystals with orientation ⟨1 1 1⟩ and it is negative (compression is easier than tension) for ⟨1 0 0⟩ single crystals. Having assumed that a plate is a primary element of the martensite structure, they explained these phenomena by the two factors: the presence of the {1 1 0}⟨1 1 1⟩ crystallographic texture in the polycrystals and the unidirectional nature of shear produced by a martensitic plate. Besides, they have pointed out that the phase deformation is affected by the different energy of coupling of martensitic plates with different habit planes and shear directions.

Authors developing macroscopic models of the mechanical behavior of SMA (e.g. works [3–5]) proposed to describe the tension–compression asymmetry by introducing the third invariant of the stress tensor into a model of the mechanical behavior of SMA. In [3,4] the pseudoelastic flow rule is formulated in terms of an equivalent stress depending on the third invariant of the stress tensor and the authors of work [5] proposed a decomposition of the transformation strain into a weighted sum, the terms of which are related to tension, compression and shear, and the weights depend on the third invariant of the stress. These works being very useful for describing the mechanical behavior of SMA do not explain the observed deformation phenomena.

The present work offers an explanation of the tension–compression asymmetry of the TiNi phase deformation due to the direct transformation on cooling. For this purpose a microstructural model [6] previously developed by the authors is used. The model assumes that the primary element of the martensite structure is a domain originated by one of the variants of Bain's distortion, rather than a martensitic plate, bearing a shear. The corresponding deformation can be described by the Bain's deformation tensor D, which is the symmetrical part of the homogeneous component of the lattice distortion. Thus, the characteristics of the tensor D must first

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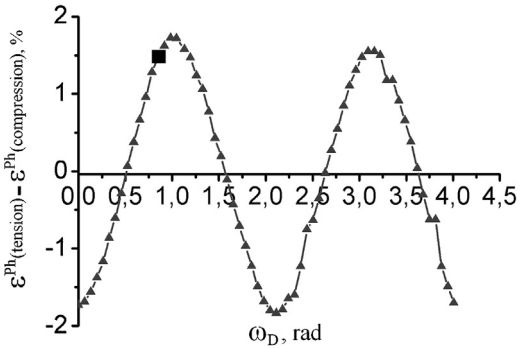

Fig. 1. Dependence of the difference between the phase deformations in tension ε^{Ph} (tension) and in compression ε^{Ph} (compression) imparted to a specimen of model material in the course of the direct transformation under stress ±100 MPa on the Bain's deformation mode angle ω_D. The square point corresponds to real TiNi.

of all influence the macroscopic deformation features of an SMA, including the tension–compression asymmetry. Being a symmetrical tensor, D can be completely specified by the orientation of its principal axes and the three invariants. The orientation of the principal axes effects the deformation of an anisotropic specimen (single crystal or a textured polycrystal), while the invariants can play a significant role in determining of the deformation of a SMA crystal independently of its orientation, and, therefore, they can affect the deformation of a polycrystal. Consider these two factors.

Crystallographic texture. For some single crystal orientations (e.g. ⟨1 1 1⟩) tension occurs at a lower stress than compression and for some other orientations (e.g. ⟨1 0 0⟩) an opposite relation is observed [1]. Since, as it was indicated in [1] the polycrystalline specimen had a crystallographic texture of the ⟨1 1 1⟩{1 1 0} type, this texture could be the reason of the tension–compression asymmetry.

First and third invariants of the lattice deformation tensor. The mechanical part of the thermodynamic driving force F_n^{mech} for the n-th crystallographic variant of the martensitic transformation is $F_n^{mech} = \sigma : D_n$ where σ is the stress tensor and D_n is the tensor of the n-th variant of the deformation due to the transformation. If D_n and σ have common principal axes, then

$$F_n^{mech} = \sigma : D_n = \left(\frac{1}{3}\right) \mathrm{Sp}\sigma\, \mathrm{Sp}D + T_\sigma \Gamma_D \cos(\omega_\sigma - \omega_D),$$

where Spσ and SpD are the first invariants (traces) of the tensors σ and D_n, T_σ and Γ_D are their second invariants (intensities of the tangential stresses and of shear deformations), ω_σ and ω_D are their third invariants (stress and strain mode angles). This formula shows that the second invariant Γ_D just determines the absolute value of the driving force, while the first and the third invariants introduce corrections dependent on the stress mode.

2. Theory/calculation

The microstructural model [6] used for simulations in this work assumes that a representative volume (point on the macrolevel) consists of grains, inside of which (on the microlevel) there can develop domains of martensite belonging to different orientation variants of the Bain's deformation. The phase macrodeformation ε^{Ph} is calculated by averaging of the microdeformations delivered by all variants inside each grain: $\varepsilon^{Gr\,Ph} = (1/N)\sum \Phi_n$ and then – by averaging of the deformations of all grains of the representative volume $\varepsilon^{Ph} = \sum \varepsilon^{Gr\,Ph}(\omega)$. Here $(1/N)\Phi_n$ are the volume fractions of different variants of martensite. The laws for the martensitic transformation are established from the balance of the thermodynamic forces, namely the chemical and mechanical driving forces, forces due to elastic interaction of martensite and austenite and

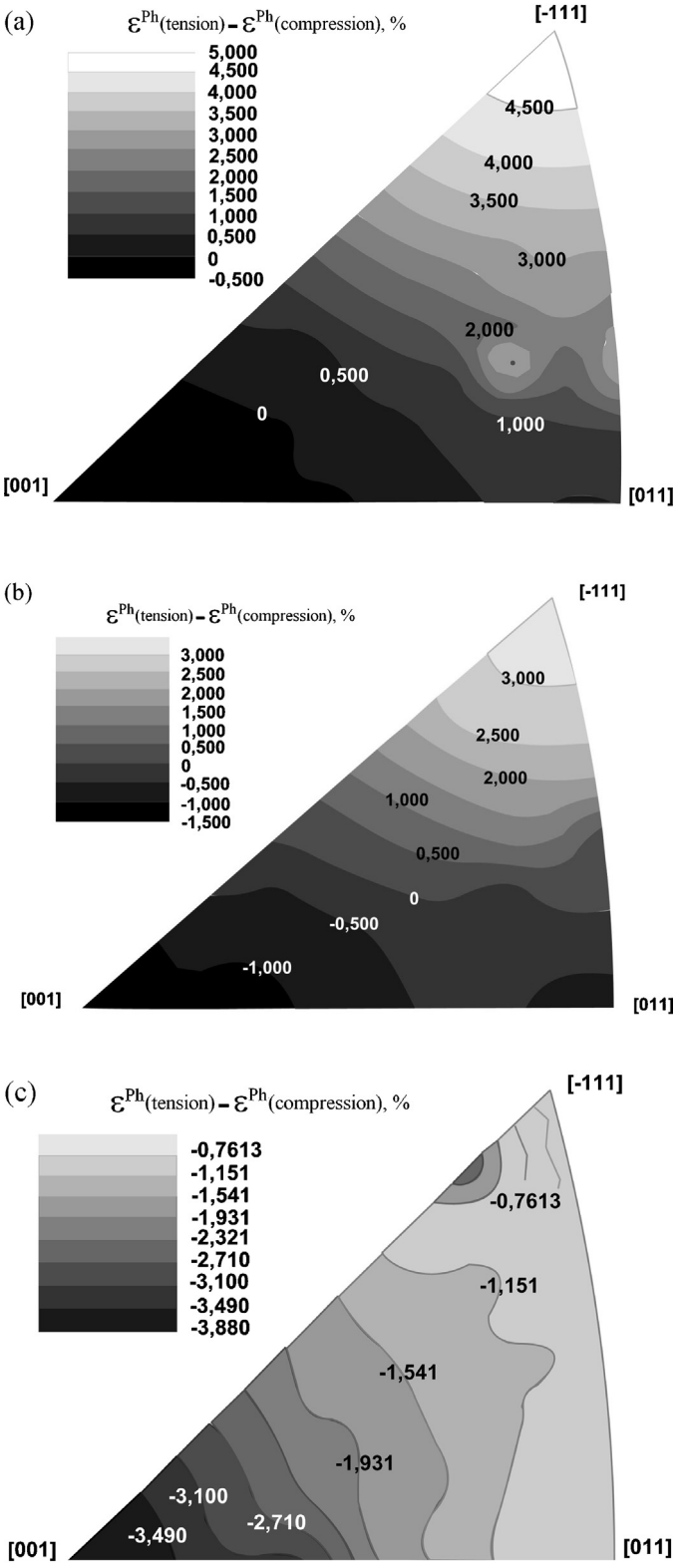

Fig. 2. Orientation dependences of the difference ε^{Ph} (tension) – ε^{Ph} (compression) on cooling of the model material single crystals with Bain's deformation mode angle: (a) $\omega_D = 0.87$ ("real" material), (b) $\omega_D = 0.59$ and (c) $\omega_D = 0$.

the dissipative "friction" force responsible for the hysteresis of the transformation.

As the first invariant of B2 → B19′ transformation is small (about +0.08%) one must conclude that it is the third invariant that determines the peculiarities of the mechanical behavior of TiNi. To make