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Influence of the twin microstructure on the mechanical properties in magnetic shape memory alloys

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ABSTRACT

The microstructure evolution, i.e. reorientation of martensite variants, is an important deformation mechanism in shape-memory alloys. This microstructure evolution occurs by the motion of twin boundaries and the nucleation and annihilation of twins in the hierarchical microstructure. An appropriate discrete disclination model for the description of the internal elastic fields and microstructure evolution is introduced for representative volume elements. The model is applied to an experimentally characterized microstructure, i.e. conjugation boundary, and the predicted mechanical response is verified by comparison to experimental measurements. The influence of the twin microstructure on the homogenized stress-strain curve is studied. It is found that regular twinned microstructures have a low strain energy and a high resistance against deformation. These simulations also reason the origin of the microstructural stability of conjugation boundaries.

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1. Introduction

Magnetic shape-memory alloys (MSMA) are technologically relevant because of their exceptional property to perform a magnetic-field-induced giant shape change. In 1996, Ullakko et al. [1] showed a magnetic-field-induced strain (MFIS) of 0.12% in a Ni_2MnGa single crystal. MFIS is based on the rearrangement of crystallographic domains to reduce the Zeeman energy. Due to the magnetic anisotropy of the martensitic phase, twin variants grow whose easy magnetization axis is aligned with the applied magnetic field. MFIS has been increased to 6% in 2000 [2] and 9.5% in 2002 [3] by microstructure optimization. It was found that the mechanical properties of Ni_2MnGa MSMA are determined by the microstructure, which is composed of different martensite variants and their twins [4].

Commonly, the non-modulated structure (NM), the 10-layered modulated structure (10 M) and the 14-layered modulated structure (14 M) are observed in the martensitic structures of NiMnGa alloys [5]. The maximum MFIS is 10% in case of a 14 M structure and 6% in case of a 10 M structure. 12% MFIS was reported by Sozinov et al., in 2013 for NM Ni-Mn-Ga-Co-Cu [6]. However, the stress induced strain of the NM structure is the highest (≈20%) [7] compared to the other structures.

The maximum MFIS is realized in case of an initial single-variant state. Magneto–thermo–mechanical training biases the twin microstructure [8], leading to a predominant twin variant; whereas very effective training leads to the formation of a single-variant crystal [9]. Untrained, self-accommodated martensite is composed of a hierarchically twinned microstructure, where higher-order, smaller twins form within lower-order twins [4,10]. It has been observed experimentally that samples that underwent effective training and that initially show large MFIS tend to fail by mechanical fatigue after a moderate number of cycles. Samples with less effective training and reduced initial magnetic-field-induced strain tend to sustain larger numbers of magneto–mechanical cycles [9].

As pointed out above, the microstructure and the capability to rearrange the microstructure are crucial for the macroscopic properties. Upon mechanical loading, the microstructure is rearranged such that the nearest neighbor relationships of atoms are maintained. When the material is heated and undergoes the

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reverse transformation back to the austenite phase, each atom "remembers" its original position and the original shape is regained [4]. The domain rearrangement is controlled by twin boundary motion. At the atomic scale, twins grow or shrink by the motion of twinning disconnections [4,11,12]. Disconnections are interfacial defects with dislocation and step character [13,14]. The dislocation step does not comprise a full lattice vector, which is referred to as partial dislocation [15,16]. In NM-martensite, the twinning disconnection step height h is the d-spacing of (202) planes and h is in the order of 2 $Å$ [16]. Since there is one twinning disconnection per step height h, the number of twinning disconnections depends on the twin thickness. If the twinning disconnections are blocked at a barrier, e.g. an obstacle twin, the twin intersection model applies here: twinning disconnection walls are represented by disclination dipoles [12,17,18]. An alternative twin mechanics model places dislocations on the twin boundary and simulates twin growth by the synchronous motion of all dislocations along the boundary. Disclination dynamics apply to both interpretations (e.g. Ref. [19]). Disclination plasticity and dynamics have been the topic of a number of recent studies, e.g. Refs. [20,21]. Here, we model the elastic fields of incoherent segments of twin boundaries as disclination dipoles. An isolated, straight truncated compound twin in its matrix is modeled by a disclination quadrupole and thousands of disconnections are simplified by using the length scale independent disclination simplification.

The characterization of the microstructure of NM Ni_2MnGa revealed that there are two types of lower-order twin boundaries: inter- and intra-variant twin boundaries [22,23]. Inter-variant twin boundaries separate different NM martensite variants and an intra-variant twin boundary separates two domains which are composed of the same martensite variant, but this variant has twinned along different twinning planes. The latter interface is referred to as conjugation boundary since both twinning systems form a conjugation pair. The lower-order twin boundaries act as glide obstacles and twinning disconnections are absorbed by these interfaces as described above. The defect content of both types of lower-order twin boundaries has been characterized experimentally [22,23]. Conjugation boundaries can be described using disclinations, whereas inter-variant twin boundaries are described by disclinations and type III Somigliana dislocations.

This paper aims to establish a quantitative relationship between twin microstructure and the mechanical properties of MSMA using discrete disclination dynamics. A discrete disclination dynamics scheme is developed in order to study the twin microstructure evolution under mechanical loading conditions. This model is applied to a twinned microstructure which comprises a lower-order hierarchical twin boundary, i.e. a conjugation boundary. We study the influence of the characteristic microstructural parameters (e.g. the twin fraction, the twin thickness and the scatter in twin thickness) on the material properties is studied. The experimental characterization of the conjugation boundary with respect to the defect content is reviewed.

2. Discrete disclination dynamics

The elastic fields of twin boundaries segments are modeled as disclination dipoles, whereas a disclination quadrupole describes a finite twin in its matrix. A discrete disclination dynamics program has been developed to model twin microstructure evolution and the governing equations will be given subsequently.

The mutual interactions of disclination dipoles as well as the behavior of disclination dipoles due to an applied load determine the twin kinetics. In Fig. 1, disclinations $\mathbf{D}_3$ and $\mathbf{D}_4$ form a dipole and the shear stress distribution $\sigma_{xy}(\mathbf{x})$ along the dipole line governs the force F_x on the dipole [24]:

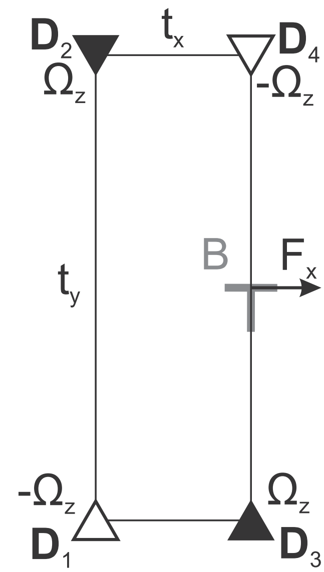

Fig. 1. Disclination quadrupole. The force F_x acts on the disclination dipole which is composed of $\mathbf{D}_3$ and $\mathbf{D}_4$. The gray dislocation symbol corresponds to the interpretation of the disclination dipole as a super dislocation.

$$F_x = L_z \Omega_z \int_{\mathbf{D}_3 \mathbf{e}_y}^{\mathbf{D}_4 \mathbf{e}_y} \sigma_{xy}(\mathbf{x}) \mathrm{d}y \tag{1}$$

where Ω_z is the disclination strength, L_z denotes the thickness in z-direction and e_y is the vertical y-coordinate. The total stress $\boldsymbol{\sigma}(\mathbf{x})$ is the sum of internal stress field and the applied load. The internal stress field is calculated by superposition of the analytical expressions for an infinitely isotropic and homogenous medium [24,25].

The force F governs the disclination dipole motion according to a linear drag relation:

$$\mathbf{F} = B\dot{\mathbf{x}} \tag{2}$$

where $\mathbf{x}$ is the disclination dipole position, $\dot{}$ denotes the time derivative and B is the drag coefficient. According to this model, the disclination quadrupole grows/shrinks in one direction and remains of constant height. This model is supported by TEM observations which depict that the dipole height remains constant along the lower order twin. Additionally, a width change is energetically much favorable compared to the height change due to the quadruple geometry. Moreover, the height change is impossible, since the conjugation boundary is blocking the disconnections as the crystallographic orientation differs on the other side. An explicit forward-Euler approach is used to determine the new position of a disclination dipole based on the dipole velocity. Moreover, the two disclinations move identically as they remain a dipole. Disclination dipoles annihilate if the separation between two dipoles with opposite sign becomes zero and the twin is annihilated. If the separating twin is annihilated, two disclination quadrupoles merge and form a joint single quadrupole.

Disclination dipole motion is restricted by a movement threshold:

$$|\mathbf{F}_x| > |\mathbf{F}_p| = \tau_p |\mathbf{B}| L_z = \tau_p t_y \Omega_z L_z \tag{3}$$

where F_p is the disclination dipole threshold-force, τ_p is threshold stress similar to the dislocation Peierl's stress, $\mathbf{B}$ denotes the

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