Influence of the Twin Microstructure on the Mechanical Properties in Magnetic Shape Memory Alloys

Benjamin Reinholz^{a,b}, Steffen Brinckmann^{a,b,*}, Alexander Hartmaier^a, Brittany Muntifering^c, William B. Knowlton^c, Peter Müllner^c

^a*Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Universitätsstr. 90a, 44789, Bochum, Germany*

^b*Max-Planck-Institut für Eisenforschung, Max Planck Str. 1, 40237 Düsseldorf, Germany*

^c*Boise State University, Boise, Idaho, USA*

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.

Keywords: Magnetic Shape-Memory Alloys, Ni₂MnGa, Twin Boundary Motion, Discrete Disclination Dynamics, Microstructural Modelling

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 Ni₂MnGa 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 Ni₂MnGa 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 (10M) and the 14-layered modulated structure (14M) are observed in the martensitic structures of NiMnGa alloys [5]. The maximum MFIS is 10% in case of a 14M structure and 6% in case of a 10M 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 ($\approx 20\%$) [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

*Corresponding author
Email address: brinckmann@mpie.de
(Steffen Brinckmann)

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 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 $2 \text{ \AA}$ [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. [19]). Disclination plasticity and dynamics have been the topic of a number of recent studies, e.g. [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 modelled 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

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

The elastic fields of twin boundaries segments are modelled 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 figure 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]:

$$F_x = L_z \Omega_z \int_{\mathbf{D}_3 \mathbf{e}_y}^{\mathbf{D}_4 \mathbf{e}_y} \sigma_{xy}(\mathbf{x}) dy \quad (1)$$

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:

$$\mathbf{F} = B \dot{\mathbf{x}} \quad (2)$$

where $\mathbf{x}$ is the disclination dipole position, $\dot{\cdot}$ 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:

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

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 Burgers vector of the super dislocation representation of a disclination dipole according to figure 1, and t_y is the twin length in y-direction. The existence of the movement threshold is reasoned by micromechanics. A straight truncated twin grows or shrinks by the amount h if a twinning disconnection moves along the twin boundary and is attached to or detached from the two disconnection walls. Since the internal resolved shear stress changes its sign along the twin boundary, twinning disconnections are trapped in regions where the resolved shear stress is zero. An applied load is necessary to overcome these traps and to proceed with disconnection motion. Furthermore, a disconnection wall is a stable configuration and a certain stress is necessary for a disconnection to escape this wall. In case of twin growth, a new disconnection dipole has to be nucleated and, for this purpose, a nucleation criterion has to be fulfilled. Therefore, the disclination dipole movement threshold stress τ_p is implemented to account for these effects.

Twin boundary motion is accompanied by plasticity that proceeds by multiple defect motion. The plastic shear γ_{xy} of a moving disclination dipole is derived analogously to Orowan's equation of a moving dislocation:

$$\gamma_{xy} = \frac{\Omega_z t_y \Delta \mathbf{x}}{L_x L_y} \frac{\mathbf{B}}{|\mathbf{B}|} = \frac{\mathbf{B} \Delta \mathbf{x}}{L_x L_y} \quad (4)$$

where L_x and L_y are the dimensions of the homogenized area. The factor $\mathbf{B}/|\mathbf{B}|$ takes account for the algebraic sign of the plastic shear and Δx is the average motion of the mobile disclinations.

3. Conjugation boundary

This section deals with the experimental characterization of a twinned intra-martensitic interface and its disclination modelling. The experimental framework conditions are given here because MSMA differ significantly by processing parameters. A single crystal has been grown by the Bridgeman method: the crushed material has been heated to 1200 °C and cooled slowly from one container end, at which a seed was located. After single crystal growth, the material has been annealed at 950 °C for 48 h and at 750 °C for 48 h. The material has been characterized as non-modulated crystal structure below the martensite finish temperature ($T < T_{Mf}$). Details on crystal growth are

provided in [26] and the experimental characterization is described in detail in [22, 23].

3.1. Experimental characterization

A transmission-electron microscope (TEM) image of an intra-martensite boundary is shown in figure 2. The diffraction patterns from domain *A* and *B* are inlaid, along with the diffraction pattern covering both domains. Crystallographic analysis [16, 22, 23] reveals that both domains are a composite configuration of the same principal martensite variant M_ξ and of parallel twins. We use the twinning nomenclature given in figure 3 (a). In domain *A*, variant M_ξ has twinned along the $(\bar{1}10)$ plane. Similarly, variant M_ξ has twinned along the (110) plane in domain *B*. Twins T_ξ^{110} and $T_\xi^{\bar{1}10}$ are compound twins of M_ξ . They are referred to as conjugation twins and conjugation boundary, because both twinning systems *A* and *B* form a conjugation pair.

The diffraction pattern over both domains shows that there is an additional misorientation. This additional misorientation is imposed by the impinging twins and effects the crystal orientation of the martensite variant M_ξ and of both twins T_ξ^{110} , $T_\xi^{\bar{1}10}$ [23]. The composite domain *A* is rotated by an angle $\tilde{\varphi}/2$ in the mathematical positive sense while domain *B* is rotated by $\tilde{\varphi}/2$ in the mathematical negative sense. Since the principal martensite variant M_ξ is rotated in both domains, each with a different sense of rotation, the superscripts “+” and “-” are added to distinguish both sections and account for their orientation.

Figure 3 (a) illustrates the different variants and their crystal orientation. The angle ψ is the angle between the twinning planes of the system M_ξ^- / T_ξ^{110} and $M_\xi^+ / T_\xi^{\bar{1}10}$. In figure 2, ψ is equal to $88^\circ \pm 1^\circ$ and the twin fraction is equal to $f_t = 0.38 \pm 0.05$. The conjugation boundary consists of a step like structure and of straight and of inclined segments. The straight segment is shown in figure 3 (a) on the left hand side and is referred to as asymmetrical facet Γ_A of a conjugation boundary [22]. Twinning disconnections join the conjugation boundary, which appears as a glide obstacle and disconnections pile up there. A symmetrical facet Γ_S of the conjugation boundary is shown in the top right corner of figure 3(a). Twinning disconnections

of both variants with Burgers vectors $\mathbf{b}_{110}$ and $\mathbf{b}_{\bar{1}10}$ meet at this interface and react with each other to form a dislocation with Burgers vector $\mathbf{b}_{100}$.

Walls of twinning disconnections shown in figure 3 (a) are simplified by disclination dipoles in figure 3 (b). Both descriptions are equal with respect to the elastic fields. As outlined in section 2, a compound twin within a matrix is described by a disclination quadrupole. According to figure 3 (b), only one disclination dipole of each twin is located at the conjugation boundary. The topology of the second disclination dipole is not resolved in figure 2, but it influences the mechanical properties. These second dipoles of each quadrupole are located at other glide obstacle in the interface vicinity. The different approaches for the conjugation boundary vicinity originate from different microstructure models.

3.2. Modelling

The conjugation boundary is modelled as a periodic structure and the elastic fields are calculated from disclination theory. We simplify the geometry to reduce the model complexity. Experimental characterization of the conjugation boundary has revealed that the twin fraction f_t determines the angle ψ between the twinning planes of both domains. Here, we assume ψ is constant (90°). This simplification entails that the Burgers vectors of the twinning disconnections are perpendicular to the interface.

Two types of facets have been identified experimentally in the interface: symmetric and asymmetric ones; the latter type is predominant [22]. Despite the fact that symmetric facets are energetically favorable in some cases, the predominance of asymmetric facets arises from kinetic reasons. In order to form an symmetric conjugation boundary, each pair of abutting twins from domains $(M_\xi^+, T_\xi^{\bar{1}10})$ and (M_ξ^-, T_ξ^{110}) have to have the same thickness and meet in registry [22]. Furthermore, the reaction of twinning disconnections from both domains is only energetically favorable if $\psi < 90^\circ$ according to Frank’s rule [27]. In this work, ψ is 90° and the disclination reaction is energetically invariant. Therefore, we only consider asymmetric boundaries because they are kinetically more probable.

Twins T_ξ^{110} and $T_\xi^{\bar{1}10}$ exhibit different crystallographic orientations. In the current model, these orientations do not influence the elastic fields, since we assume an isotropic material. The twin color

⁰Figure 2: Reprinted from Acta Materialia with permission from Elsevier.

Figure 2: Transmission electron micrograph of a conjugation boundary separating two domains. Domains are composed of the same martensite variant which has twinned along different twinning planes. Twins in domain A and B are conjugate twins [22].

scheme is changed from red/blue (figure 3) to blue (figure 4) to emphasize the isotropy assumption.

The model goal is to simulate an infinite periodic structure. Analytical elastic solutions for periodic disclinations only exist in special cases [28, 29]. For general two dimensional configurations, no analytical expressions exist. Therefore, a quasi-periodic approach is used here which is similar to dislocation approaches like the infinite body solutions for dislocation strings [30] and for a periodic simulation cell [31]. The elastic fields are calculated for a representative volume element (RVE) as shown in figure 4: n images of the RVE extend in all directions. The elastic fields are calculated by the superposition of analytical expressions of the disclinations from within the RVE and their $(2n+1)^2 - 1$ images. The total stress state is the superposition of the internal disclination stresses and the applied load. The elastic fields at point $\mathbf{P}$ are:

$$\sigma(\mathbf{P}) = \sum_{j=-n}^n \sum_{k=-n}^n \sum_{i=1}^{n_d} \sigma(\mathbf{X}_i(j, k), \Omega_z^{(i)}) \quad (5)$$

$$\mathbf{X}_i(j, k) = \mathbf{P} - \mathbf{D}_i - \begin{pmatrix} jL_x \\ kL_y \end{pmatrix} \quad (6)$$

where $\sigma(\mathbf{P})$ is the internal stress tensor at point $\mathbf{P}$, n_d denotes the number of disclinations, $\sigma(\mathbf{X}_i, \Omega_z^{(i)})$ is the stress function [24], $\mathbf{D}_i$ denotes the position of the i -th disclination, $\mathbf{X}_i(j, k)$ is the relative position of the i -th disclination / their periodic image to point $\mathbf{P}$. L_x and L_y are the characteristic lengths

of the RVE. Stress functions also depend on the disclination strengths Ω_z .

The finite RVE area and its images is surrounded by one disclination quadrupole with variable strength. The correction disclination strength depends linearly on the twin fraction [32]:

$$|\Omega_z^{Cor}| = \Omega_z f_t \quad (7)$$

The correction quadrupoles alter the outer infinite variant such that the RVE is embedded into a matrix with the same twin fraction as the RVE.

The periodic step-like character of the conjugation boundary RVE leads to rectangular domains as illustrated in figure 4. These rectangular domains are referred to as cells. The disclination dipole motion is restricted by their cell topology. The twin thickness scatter is described by the irregularity θ : the initial disclination dipoles positions are altered by a random value along their glide direction:

$$\Delta_{\bar{x}} = \kappa \lambda_t \theta \quad (8)$$

where $\Delta_{\bar{x}}$ is the initial dipole displacement, κ denotes a random number within $-1 \leq \kappa \leq 1$ and λ_t is the initial twin thickness.

3.3. Material parameters and numerical implementation

We simulate a RVE of $L_x = 1\mu\text{m}$, $L_y = 1\mu\text{m}$ and employ an isotropic elastic shear modulus of $G = 4\text{GPa}$ [33] with a Poissons ratio of $\nu = 0.3$.

Figure 3: Crystallographic interpretation of the conjugation boundary. Domain A is composed of martensite variant M_ξ^+ and its compound twin T_ξ^{110} , whereas variant M_ξ^- and its compound T_ξ^{110} is present in domain B. (a) Twinning disconnections pile up at the conjugation boundary. (b) Twinning disconnection walls at the interface are simplified by disclination dipoles. Schematic (b) depicts a larger area than schematic (a).

The disclination strength is $\Omega_z = 0.3344\text{rad}$ [22] and the annihilation distance $l_{\min} = 1\text{nm}$, i.e. if the twin thickness decreases below this value, the twin is removed from the simulation. The threshold stress for disclination motion is assumed 20MPa and the drag coefficient is $B = 1000\text{Pa s}$. The time increment is 0.25s and the maximum applied stress is 50MPa . Figures are rendered with at least 200 points in each direction.

The numerical implementation is based on the formulation of stress fields. Within each loading step, the applied stress is increased and superposed on the internal stresses arising from the disclinations. The thus-obtained resolved shear stress on each disclination dipole and the time step dictate the disclination motion according to the Forward Euler method. In the new disclination position, the updated internal stress distribution is evaluated and used to relax the disclination distribution. The relaxation is stopped once the maximum motion of a disclination drops below the threshold distance 10^{-9} times the twin thickness. After the disclination distribution is relaxed, the corresponding shear strain is evaluated by the distance of disclination motion based on their initial position resolved on the disclination motion plane. The shear strain is superposed to the applied shear strain according to Hooke's law. This calculation finalizes the loading step. The applied load is increased and the pro-

cedure started again until the maximum applied stress is reached. The unloading behavior is purely elastic, because no disclinations are in the domain at that point.

4. Results

4.1. Internal elastic energy

In this section, we investigate the influence of the twin microstructure on the elastic state. The specific elastic energy is shown as function of the twin fraction f_t and the number of twins per cell n_t (figure 5 (a)) and as function of the irregularity θ (figure 5 (b)). The elastic energy e as function of the number of twins n_t and twin fraction f_t is shown only for $f_t \leq 0.5$ because the elastic energy symmetrical about the maximum at $f_t = 0.5$. The energy increases non-linearly with the twin fraction and decreases hyperbolically with the number of twins. The irregularity is increased incrementally in 0.1 steps from $\theta = 0.0$ to $\theta = 2.0$. The energy is shown for eight random microstructures for each θ . Regular structures have a lower energy than irregular ones. The elastic energy of irregular structures ($\theta = 2$) is approximately five times higher than the elastic energy of regular structures. Moreover, the spread of the specific elastic energy e increases with increasing the irregularity θ .

Figure 4: The conjugation boundary is modelled as a RVE. Disclination images are created by copying the RVE disclination configuration n times in all directions. Furthermore, a correction quadrupole is added at the periphery that results in the same twin fraction in the outer infinite variant matrix.

4.2. Kinetics

The homogenized stress strain behavior of a twinned microstructure is studied in this section. The applied stress is increased linearly with time and is superimposed on the local disclination stress. A tensile load is applied in ξ -direction that is inclined by 45° with respect to the horizontal x -axis. The shear stress on the disclination dipoles drives the kinetics, hence the responses in tension and compression are symmetrical. The twin microstructure is relaxed for each load increment, i.e. the dipoles are stable.

Initially, we study in detail the evolution of one twinned microstructure. Afterwards, we present the influence of the initial twin fraction (f_t), the disclination movement threshold (τ_p) the number of twins per cell (n_t) and the irregularity of the twin thickness (θ) on the homogenized stress strain curves.

4.2.1. Microstructural evolution

The stress strain curve of an irregular microstructure ($n_t = 10$, $\theta = 1$, $f_t = 0.5$ and $\tau_p = 20$ MPa) is shown in figure 6. The shear stress distribution with respect to the xy -coordinate system and the disclination evolution are inlaid.

In the first section of the stress strain curve, the linear elastic relationship is accompanied only

with minor plastic deformation. Thereafter, the hardening rate is degressive until the stress reaches 25 MPa. Subsequently, a wide stress plateau exists in which most plastic deformation occurs. Then, the stress increases progressively until it reaches 40 MPa, which is $2\tau_p$. Finally, the stress strain relationship is linear elastic again.

The applied load case favors the martensitic matrix: as the load increases, twins shrink and annihilate finally. During the initial linear elastic section the twin structure does not change significantly. Only thick twins thin down during the degressive region (up to point (b)), whereas thin twins remain stable. During the stress plateau (≈ 25 MPa), substantial twin boundary motion takes place ((b) $\rightarrow$ (c)): thick twins and thin twins shrink. The twin microstructure relaxes as all twins reach a similar thickness. The twins thin down further within the progressive section ((c) $\rightarrow$ (d)). Finally, all twins are annihilated and a single crystal remains. This single crystal is composed of martensite variant M_ξ . Further loading results in a linear elastic response.

Tension in ξ -direction leads to a positive shear stress in the RVE with respect to the xy -coordinate system. In the first increment, the applied load is zero and the total stress state (figure 6 (a)) is only determined by the internal stresses. Regions

Figure 5: (a) Specific elastic energy e as function of the twin fraction f_t and the number of twins n_t . The irregularity $\theta = 0$. In case of $f_t = 0.5$, the specific energy scales with $n_t^{-1.15}$ ($C_1 = 9.224 \text{ MJ/m}^3$). (b) Specific energy e as a function of the irregularity θ . The number of twins $n_t = 10$ and the twin fraction $f_t = 0.5$.

of positive and negative shear stress are equally distributed. The stress state in the elastic and in the degressive region is unstructured. Stresses in the interface vicinity exceed the stress bar bounds. As the applied load increases, regions of negative shear stress decrease in size and magnitude. Even though the superimposed shear stress is positive, the shear stress does not increase everywhere in the RVE: the circled region in figure 6 (a) exhibits a high shear stress. This stress decreases even with increasing applied load ($(a) \rightarrow (d)$). The twin structure in this region is altered during this process from an irregular (high internal stresses) to a regular structure (low internal stresses). Local excess stresses diminish as twin boundaries move. At the onset of the progressive region, the internal disclination stresses decrease and the stress state is dominated by the applied load.

4.2.2. Influence of the microstructure on the stress-strain curve

The influence of the initial twin microstructure on the global stress-strain behavior is studied in this section. The resulting stress-strain curves are shown in figure 7 for tensile loading in the ξ -direction.

The influence of the initial twin fraction f_t on the homogenized stress-strain curve is studied in figure 7 (a). The plastic transformation strain as well as the twinning stresses¹ increase with the initial twin

¹The twinning stress is the stress at which distinct twin boundary motion takes place and marks the onset of plastic deformation.

fraction. For each case with $f_t \leq 0.5$, the progressive region ends at $40 \text{ MPa} = 2\tau_p$ and for the cases $f_t > 0.5$, the twinning stress exceeds $2\tau_p$. The stress strain curves depend also qualitatively on the initial twin fraction. The degressive region flows smoothly into the progressive region without stress plateau in case of $0.1 \leq f_t \leq 0.2$. The stress strain curves exhibit the sequence elastic region, degressive region, stress plateau, progressive region and elastic region as presented in the previous detailed analysis, if the initial twin fraction is in range of $0.3 \leq f_t \leq 0.5$. If the initial twin fraction is higher than 0.5, the degressive region is followed by the stress plateau and no progressive region is present.

In figure 7 (b), the disclination dipole movement threshold τ_p is varied. In case of no movement threshold (red color code in figure 7 (b)), the initial disclination configuration is unstable. In this case, disclination quadrupoles adjust themselves due to the internal stress state and the initial twin configuration evolves. All remaining twins disappear during the first load increment. In the other cases $\tau_p > 0$, the stress strain curves resemble each other quantitatively. The curves are scaled by the movement threshold which correlates with the twinning stress.

In figure 7 (c), the initial number of twins per cell n_t is varied. The initial microstructure is unstable in case of low numbers of twins per cell. In this case, disclination quadrupoles adjust themselves to the internal stress state. Those twins which are located in the corner of a cell shrink in the first time increment. This adjustment of the initial twin microstructure reduces the achievable plastic trans-

Figure 6: Stress strain curve of an irregular twinned microstructure. The shear stress with respect to the xy -coordinate system and the disclination structure are inlaid.

formation strain. The initial configurations become more stable as the number of twins per cell increases. However, the twinning stress increases with the number of twins per cell and approaches the disclination movement threshold stress for fine twinned microstructures. Moreover, stress strain curves change qualitatively in dependency of the number of twins per cell. They exhibit the prior described features of degressive region, stress plateau and progressive region in case of coarse twin structures. The stress plateau becomes dominant at the expense of the other two regions as the microstructure is finer twinned.

In figure 7 (d), see equation (8). The total achievable plastic strain varies for different irregularities. More homogeneous microstructures reach a higher plastic strain. The presented results show only tendencies of the influence of the irregularity. The stress strain curves scatter for the same irregularity θ due to the random nature. Generally, irregularly twinned microstructures exhibit a lower twinning stress than regular structures. There is a wide scatter in the stress strain curves for high θ . In cases of high irregularities, the twinning stress drops and the degressive and progressive regions of the stress strain curve become more dominant at the expense of the stress plateau. In case of excessive irregu-

larities, the twinning stress drops further and some stress strain curves exhibit no stress plateau at all, e.g. $\theta = 1.5$.

4.2.3. Summary

Five different characteristic sections of the homogenized stress-strain curve are identified:

- i) elastic region: The material follows the linear elastic Hooke's law. No twin boundary motion occurs.
- ii) degressive region: The stress increases degressively with strain. Thick twins thin down, whereas thin twins remain stable. Thick twins cause high local stresses, which are reduced in this process.
- iii) stress plateau: Distinct plastic strain occurs within a small stress range. Excessive twin boundary motion takes place. Thick and thin twins decrease in width until the microstructure becomes regular with almost equidistant small twins.
- iv) progressive region: The stress increases progressively with increasing strain. Small equidistant twins diminish further until they annihilate finally. Local stress disturbances

Figure 7: Influence of model parameters on the homogenized stress-strain curve. a) Vary initial twin fraction f_t ; while keeping twin number $n_t = 10$, irregularity $\theta = 0$ and movement threshold $\tau_p = 20$ MPa constant. b) Vary movement threshold τ_p ; while keeping twin number $n_t = 10$, initial twin fraction $f_t = 0.5$ and irregularity $\theta = 0$ constant. c) Vary twin number n_t ; while keeping initial twin fraction $f_t = 0.5$, irregularity $\theta = 0$ and movement threshold $\tau_p = 20$ MPa constant. d) Vary irregularity θ ; while keeping initial twin fraction $f_t = 0.5$, twin number $n_t = 10$ and movement threshold $\tau_p = 20$ MPa constant.

vanish and the stress state within the RVE is dominated by the applied load. For each case with $f_t \leq 0.5$, the stress at which detwinning completes equals $2\tau_p$ and for the cases $f_t > 0.5$, the twinning stress exceeds $2\tau_p$.

- v) elastic region: The material behaves according to Hooke's law. The material consists of a single domain.

The above described sections of the stress strain curve are also observed in experimental tests as detailed subsequently and according to [7].

Irregularly twinned microstructures exhibit a lower twinning stress. Furthermore, the degressive and progressive regions of the stress strain curves are more pronounced. In these cases, the stress plateau is less pronounced and is absent for large disorder. Irregularities in the twin thickness lead to high local stresses in the vicinity of the inter-

face, which is accompanied by a lower resistance against plastic deformation.

5. Discussion

5.1. Discussion simulation

The present twin microstructure model of a conjugation boundary does not allow for conjugation boundary motion. Instead, mechanical loading reduces the twin fraction f_t which is accompanied by the eventual conjugation boundary dissolution and the evolution of a single crystal. **Two step-wise parallel conjugation boundaries are present for periodic reasons in the RVE. There is a limited interaction between both boundaries initially, as highlighted by the stress contours in Fig. 6(circled area). The interaction between both boundaries vanishes during and after the strain plateau. Hence, the conjugation**

Figure 8: Specific elastic energy e of a twinned microstructure as function of the twin fraction f_t and its negative derivative $-de/df_t$ which represents the driving force of the system. The internal driving force is used to explain the features of the homogenized stress strain curve.

boundary interaction is insignificant for the simulation result.

The number of twinning disconnections in the conjugation boundary increases linearly with the twin fraction f_t . Furthermore, the elastic energy e is bell-shaped with respect to the twin fraction f_t (figure 8). If $f_t > 0.5$, the elastic energy e decreases with increasing twin fraction f_t even if the number of twinning disconnections and the disconnection density increases. This conjugation boundary feature arises from the step-like pattern of the asymmetric facets because the stress and strain fields of such arranged twinning defects reduce each other.

The stress strain curves are discussed on the basis of figure 8, which shows the specific elastic energy of the RVE as function of the twin fraction along with its negative derivative, which represents the global driving force. The scalar global driving force $-de/df_t$ indicates the global evolution direction, while the stress state determines disclination dipoles evolution, which might evolve toward a different twin fraction. There is an internal driving force which points towards $f_t = 0.0$ if $f_t < 0.5$ and towards $f_t = 1.0$ if $f_t > 0.5$. The microstructure is in an instable equilibrium if the twin fraction is $f_t = 0.5$. If the disclination dipole movement threshold is not exceeded by the internal driving force, the microstructure is stable. Therefore, an additional applied load is necessary to induce twin boundary motion.

- Originating from an initial twin fraction of $f_t = 0.1$ (point a in figure 8) the internal

driving force points towards zero twin fraction. Disclination dipoles move if the movement threshold is exceeded by the sum of internal and external driving forces. Disclination dipole motion leads to a twin fraction decrease, thereby, decreasing the internal driving force. This force drop has to be balanced by the applied load in order to sustain twin boundary motion.

- The internal driving force points also towards twin annihilation for moderate initial twin fractions ($f_t = 0.4$, point b in figure 8). In this configuration, the internal driving force increases, if the movement threshold is exceeded by the sum of the internal and external driving forces. Therefore, disclination dipoles move continuously until point b' at constant applied loads. The unstable $b \rightarrow b'$ motion explains stress plateau existence because massive plastic strain occurs at constant applied stress. After point b' the internal driving force decreases and the applied load has to be increased to trigger further disclination motion towards $f_t = 0$. This behavior is seen as progressive regimen in the global stress strain curve. At $f_t = 0$, there is no internal driving force and, thus, $\sigma_{\xi\xi} = 2\tau_p$
- Starting with a high initial twin fraction ($f_t = 0.6$, point c in figure 8), the internal driving force points towards 100% twin fraction. The applied load has to overcome this driving force as well as the movement threshold in order to

reduce the twin volume fraction f_t . The twinning stress is therefore higher than the disclination dipole movement threshold as shown in figure 7 (a). After exceeding the movement threshold, disclination dipoles move until all twins annihilate without any further applied load increase.

In these simulations, the stress does not drop during the stress plateau, because the applied load is prescribed. If the displacement were prescribed, a stress drop is expected during the transformation plateau.

The prior described analysis is valid for regular twinned microstructures. Irregular twinned microstructures exhibit a higher strain energy which also results in higher local driving forces. Therefore, the required applied stresses are lower to trigger the stress plateau. Furthermore, the highest local stresses occur for coarse twins, which move initially and lead to a decrease in twin thickness variability and to local stress maxima disappearance.

5.2. Comparison to experiments

A series of compressive tests was performed on a non-modulated $\text{Ni}_{52.5}\text{Mn}_{26}\text{Ga}_{21.5}$ single crystal with lattice parameters $a = b = 5.506$, $c = 6.496\text{\AA}$ using a modified Zwick 1445 mechanical test bench. The single crystal was cut along 001A planes to $x = 3\text{mm}$, $y = 4\text{mm}$ and $z = 5\text{mm}$. X-ray diffraction was performed in between compressions. The intensity ratio of (004) to (040) peaks was used to approximate the fraction of twins oriented with the c axis nearly parallel to the compression direction, since these are the variants that will transform in response to the stress. Three example curves are demonstrated for multiple twin fractions. The first curve “Z” shows a compression along the z axis when the fraction of twins – oriented with their c axis parallel to the compression direction – was approximately 12%. No clear stress plateau is present, and only a small strain $< 1\%$ was achieved. This curve strongly resembles the curve in figure 7 (a) when $f_t = 0.1$ in which no clear stress plateau is present and a comparably low strain is achieved. The second curve “Y” is performed along the y axis of the sample, when approximately 30% of the variants were oriented with their c direction parallel to the applied force. This compression resulted in approximately 6% strain – with a clear stress plateau around 9.5MPa. This curve strongly resembles the

$f_t = 0.3$ curve of figure 7 (a). A final compression was performed in the x -direction of the sample, when approximately 87% of the variants were oriented with their c axis parallel to the compression direction, curve “X” in figure 9. This compression resulted in approximately 14% strain, with the stress plateau around 17MPa. The increase in stress of the stress plateau with higher twin fraction agrees with figure 7 (a).

5.3. Comparison with in-situ TEM observations

Recent in-situ TEM observations support concepts of collective and coordinated twinning events inherent to the model presented here. Zárubová et al. [34] reported the stress-induced motion of an inter-variant boundary in non-modulated Ni-Mn-Ga. In this situation, twin boundaries moved coordinated first in one martensite variant which detwinned as a result. In a second step, the twins in the other variant then propagated into the detwinned variant. The detwinning of the first variant lead to a reorientation which aligned this variant with the other variant. This is similar to the model presented here where the twinning process rotates the domains across the conjugation boundary to form a single variant (Fig. 6). Muntifering et al. [35] described in-situ TEM results of a moving conjugation boundary in Ni-Mn-Ga. Similar to the mechanism discussed here, Muntifering et al. observed the dissolution of a twin structure through an orthogonal shearing process. In both cases the orthogonal shear is carried by cooperative twinning and twin motion can be interpreted as the propagation of a disclination dipole. In the case described by Muntifering et al. secondary twinning occurs inside the twins (and matrix) of the twins forming the conjugation boundary as proposed by Müllner and King [36] and the conjugation boundary moves via a microstructural transformation which is described as a coordinated rearrangement of disclination dipoles. In contrast, the model proposed here considers primary twinning eventually leading to a dissolution of the stationary conjugation boundary. Orthogonal shearing processes similar to these reported here are found in many materials, particularly with the evolution of shear bands as described in Ref. [37]. Ge et al. [38] observed a stress induced transformation from 14M to non-modulated martensite involving cooperative twinning mechanisms. Similar to the case reported by Zárubová et al. [34], the transformation occurred with a two-step mechanism. All these mechanisms have the

Figure 9: Experimental stress-strain curves for single crystal. The compression direction is in the x,y,z axis respectively.

following features in common with the model presented here. (I) Twins move collectively, (II) twins may be represented by disclination dipoles, (III) collective twinning results in a rotation (combined with shear), and (IV) collective twinning results in the motion and/or dissolution of an internal boundary.

6. Conclusions

The present publication investigates the influence of the twin microstructure on the macroscopic mechanical properties of NM Ni_2MnGa . A numerical model has been developed to describe the elastic state and the microstructure evolution under mechanical loading for a twinned microstructure with a conjugation boundary. The developed discrete disclination model explains the features typically observed in experimental stress strain curves for shape-memory alloys. The model constructs a representative volume element by elimination of the artificial macroscopic boundary condition that is present in conventional non-periodic models.

The simulations identify five characteristic regions: the elastic regime, the degressive region, the stress plateau, the progressive region and a second elastic region. The form and extend of each region depends on the twin microstructure and the applied load. Furthermore, microstructural irregularities, such as varying twin thickness, have a significant influence on the elastic state and on the irreversible deformation: irregularly twinned microstructures have a significantly higher elastic energy and the stresses and strains are distributed without apparent order.

These microstructures exhibit a lower twinning stress than regular twinned microstructures and their progressive as well as degressive region of the stress strain curve are more pronounced. Additionally, the strain energy of the conjugation boundary depends on the twin microstructure. The strain energy is low in case of thin and equidistant twins and microstructures that exhibit a low internal strain energy have a low mobility. Conjugation boundaries are microstructural key feature for the deformation process because of their low internal strain energy and their low mobility, resulting in a high stability.

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