Numerical Simulation of Twin-Twin Interaction in Magnetic Shape-Memory Alloys

Markus Chmielus1,2, David Carpenter1, Alan Geleynse1, Michael Hagler1, Rainer Schneider2, and Peter Müllner1
1Materials Science and Engineering, Boise State University, 1910 University Dr., Boise, ID, 83725
2Diffraction Group, Dept. SF1, Hahn-Meitner-Institut, Berlin, 14109, Germany

ABSTRACT
Twin boundary motion is the mechanism that drives the plastic deformation in magnetic shape memory alloys (MSMAs), and is largely dependent on the twin microstructure of the MSMA. The twin microstructure is established during the martensitic transformation, and can be influenced through thermo-magneto-mechanical training. For self-accommodated and ineffectively trained martensite, twin thickness and magnetic-field-induced strain (MFIS) are very small. For effectively trained crystals, a single crystallographic domain may comprise the entire sample and MFIS reaches the theoretical limit. In this paper, a numerical simulation is presented describing the twin microstructures and twin boundary motion of self-accommodated martensite using disclinations and disconnections (twinning dislocations). Disclinations are line defects such as dislocations, however with a rotational displacement field. A quadrupole solution was chosen to approximate the defect structure where two quadrupoles represent an elementary twin double layer unit. In the simulation, the twin boundary was inclined to the twinning plane which required the introduction of twinning disconnections, which are line defects with a stress field similar to dislocations. The shear stress - shear strain properties of self-accommodated martensite were analyzed numerically for different initial configurations of the twin boundary (i.e. for different initial positions of the disconnections). The shear stress - shear strain curve was found to be sensitive to the initial configuration of disconnections. If the disconnections are very close to boundaries of hierarchically higher twins – such as is the case for self-accommodated martensite, there is a threshold stress for twin-boundary motion. If the disconnections are spread out along the twin boundary, twinning occurs at much lower stress.

INTRODUCTION AND BACKGROUND
It has been shown that MSMAs can produce a field induced strain exceeding 10% upon the application of a magnetic field, which results from moving twin boundaries driven by internal stresses produced by magnetic anisotropy energy and/or mechanical loading [1-4]. For Ni-Mn-Ga single crystals, the MFIS strongly depends on training, i.e. on thermo-magneto-mechanical treatment [5, 6]. The training biases the twin microstructure of the crystal leading to a predominant twin variant. Effective training leads to the formation of a single-variant crystal, while ineffectitive training leads to a microstructure that contains various twin variants with almost equal fractions. For effectively trained Ni-Mn-Ga, magnetic-field-induced deformation tends to be large and permanent upon removal of the magnetic field. For this type of deformation, the term ‘magnetoplasticity’ is used [7, 8]. For ineffectively trained Ni-Mn-Ga, magnetic-field-induced deformation tends to be small and the strain recovers upon removal of the magnetic field. The term ‘magnetoelasticity’ is used for this type of deformation [9].
To better understand the effect of twin microstructure on magnetic-field-induced or mechanically induced deformation, a micro-mechanistic model is necessary. From the macroscopic perspective, magnetoplasticity is the changing of shape due to a magnetic field. On the mesoscopic scale, this shape change is related to the reorientation of crystallographic twin domains. The twin domains are formed during a structural (martensitic) transformation. The reorientation of domains is mediated through the motion of twin boundaries. On the microscopic scale, the carriers of magnetoplasticity are disconnections which are line defects similar to dislocations located at coherent twin boundaries where they form incoherent steps [10, 11]. Twinning disconnections move along the twin boundaries and are driven by a magnetically and/or mechanically induced force. Disconnection motion results in a displacement of the twin boundary and shear deformation.

The presence of different twin-variants affects the mobility of twin boundaries. A very effective way to model twin-twin interaction makes use of the disclination model for twinning[12]. Disclinations are line defects similar to dislocations, however with a rotational displacement field [13]. The disclination model for twinning makes use of disclination dipoles, which have the same long-range displacement field as a dislocation wall [13].

The aim of this paper is to outline how disconnections and disclinations can be applied to develop micromechanistic models of twinning processes in multi-twin-variant microstructures and how these models can predict mechanical and magneto-mechanical properties of magnetic shape-memory alloys.

**DISCLINATION MODELS FOR TWINNED MARTENSITE**

The main contribution to the martensite transformation strain of B2-alloys results from a shear-instability on the (110)[\(\overline{1}10\)] shear system [14]. Twinning occurs on the same shear system. In a thought experiment, twinned martensite can be formed during the austenite-martensite phase transformation by growth of two martensite lamellae on the same shear plane but in opposite shear direction, e.g. on the shear systems (110)[\(\overline{1}10\)] and (110)[\(1\overline{1}0\)]. Figure 1a depicts four martensite lamellae in an austenite matrix. The shear systems are (110)[\(\overline{1}10\)], (110)[\(1\overline{1}0\)], (1\(\overline{1}0\))[\(110\)] and (1\(\overline{1}0\))[\(1\overline{1}0\)]. The two martensite lamellae on (110) form a twin double layer as do the martensite lamellae on (1\(\overline{1}0\)). Each martensite lamella has long, coherent martensite/austenite and martensite/martensite interfaces and a short, coherent interface between martensite and austenite. The short interface carries the transformation in the form of a wall of transformation disconnections or, equivalently, by a transformation disclination dipole with disclination strength \(\omega\). In Figure 1, positive and negative disclinations are displayed as solid and open triangles, respectively.

In the next step of this thought experiment, more martensite lamellae grow and form two stacks of twins (Figure 1b). At the same time, the short interfaces move towards each other and the disclinations start to interact. Positive and negative disclinations attract and cancel as they meet. There are a number of options how the disclinations may interact. One possibility is indicated with ellipses in Figure 1b, and the resulting twin-microstructure is given in Figure 1c. The displacement field is characterized by a wall of alternating positive and negative disclinations with strength \(2\omega = 2\tan^{-1}(s/2)\) which equals the twinning disclination power [15]. The parameter \(s\) is the twinning shear. A second example of the defect content of a hierarchical twin microstructure is shown in Figure 1d.
Figure 1: Twinned martensite. (a-c) Though experiment to illustrate the defect content. (a) Pairs of twinned martensite plates form on (110) and (1 \parallel 10) planes. Adjacent lamellae have opposite shear directions, e.g. the plates on (110) have shear directions [1 1 0] and [ \bar{1} 1 0]. Thus, bright and dark plates are twinned. The shear deformation is carried by the motion of disclination dipoles (i.e. a pair of solid and open triangles). (b) With ongoing transformation, the number of martensite plates increases and the dipoles move such as to extend the size of the plates. When different martensite variants meet, disclinations interact. Schematic (c) is one option of the resulting microstructure characterized by a wall of alternating positive and negative disclinations. (d) Defect content of a different hierarchically twinned microstructure. (e) Magnetic force microscopy image of martensite in a (Ni_{51}\text{Mn}_{28}\text{Ga}_{21})_{99.5}\text{Dy}_{0.5} single crystal displaying the magnetic structure which corresponds to the twin structure. (f) Transmission electron microscopy image of twinned martensite in a Ni_{51}\text{Mn}_{28}\text{Ga}_{21} single crystal displaying a twin microstructure similar to the schematic (d). P and S mark primary and secondary twin boundaries.

Figures 2e and 2f are a magnetic force microscopy (MFM) image and a transmission electron microscopy image of twinned martensite in (Ni_{51}\text{Mn}_{28}\text{Ga}_{21})_{99.5}\text{Dy}_{0.5} and Ni_{51}\text{Mn}_{28}\text{Ga}_{21} single crystals, respectively. The magnetic structure reflects the twin structure of the specimen. These images represent real cases corresponding to the schematics shown in Figures 2c and 2d.

QUADRUPOLE APPROXIMATION AND NUMERICAL SIMULATION

In reality, it is the motion of individual transformation disconnections through which martensite forms. Likewise, twin boundary motion is achieved by the motion of individual twinning disconnections. The disconnection motion is brought about by the application of a magnetic field and/or applied mechanical stress. To model this process, a numerical simulation
must take into account the individual twinning disconnections. Since the patterns in Figures 1c and 1d are too complex, the model must be simplified while still accounting for the main characteristics of the defect structure. One characteristic of a disclination wall is that at an increasing distance from the wall, stress and strain rapidly decrease and vanish [16]. Thus, a disclination wall is a self-screening disclination ensemble. A satisfactory approximation for the stress field of a disclination wall was found in disclination quadrupoles [17, 18]. A quadrupole model can also be used to study the geometry and energy of twins within twins [19], which is very similar to the twin structure observed in shape-memory alloys.

Figure 2: Quadrupole approximation of the twin-microstructure. (a) The elementary unit of a double twin layer of the pattern in Figure 1d. The double layer is bound by two vertically arranged disclination quadrupoles. In each quadrupole, the central two disclinations have the same sign and are positioned at the same location, i.e. they appear as one disclination with strength ±2ω. In (b), the corner disclinations form a rectangle. The twin boundary is inclined and, therefore, is decorated with twinning disconnections (displayed with dislocation symbols). Parameters t and l are defined as the twin thickness and twin domain width, while p = 2q/λ is the slope parameter and α is the inclination angle of the twin boundary. (c) As the disconnection moves and aligns in the vertical interface, the disclination quadrupoles establish. The central disclination with strength ±2ω moves along the vertical interface by one d-spacing when a twinning disconnection is incorporated into the vertical interface.

Figure 2a shows a double twin layer, which is represented by two disclination quadrupoles. The double twin layer is the smallest repeating unit of a twin-microstructure resulting from plates formed all on (110) planes. Each quadrupole of the double twin layer contains two positive and two negative disclinations, with a strength of ±ω. The central disclinations combine and form one disclination with a strength ±2ω. For numerical simplification, the quadrupoles are arranged such that the four corner disclinations form a rectangle. To introduce twinning disconnections, the twin boundary is rotated and is now inclined by an angle α with respect to the twinning plane. Twinning disconnections sit on each twinning plane and are represented in Figure 2b with dislocation symbols. Figure 2b represents a model for self-accommodated martensite, which can be used for numerical simulations. Since the stress field of a disconnection is the same as that of a dislocation, dislocation theory applies.

An iterative process is used to determine the equilibrium position of all disconnections. For each iteration, the net force on each disconnection is found by (i) the interaction forces with all other disconnections, (ii) the interaction forces with the disclinations, and (iii) the Peach-Koehler force due to an applied stress. Each disconnection is then displaced along the twinning plane by an amount proportional to the total force. Twinning disconnections that move into the vertical boundary defined by the two quadrupoles are removed from the twinning plane. They are incorporated into the disclination wall and cause the central disclination (±2ω) to move vertically by one interplanar spacing (Figure 2c). This process is repeated until (i) all
disconnections are incorporated into the disclination wall, resulting in their removal and disclination motion, or (ii) the total force on all disconnections is below a critical value, which is the stopping criterion of the simulation.

RESULTS, DISCUSSION, AND CONCLUSION

Several simulation series were performed to determine the influence of the initial slope of the twinning plane on the shear stress – shear strain curve. 1000 disconnections were assumed in each twin layer. The ratio of twin-domain width \( \lambda \) and twin thickness \( t \) was 10, and the twinning shear \( s \) was 0.124 (corresponding to a \( c/\alpha \) ratio of 0.94, where \( \alpha \) and \( c \) are the lattice parameters of the tetragonal 10M martensitic phase). A shear modulus of 10 GPa was assumed. The shear stress was varied from 0 to 250 MPa. The results are shown in Figure 3. If the slope parameter \( p = 2q/\lambda \) is larger than 0.2, small stresses are sufficient to induce strain. The strain increases gradually with stress. The hardening rate increases with decreasing \( p \). When the slope parameter is reduced below 0.2, the shear stress for twinning increases distinctly to above 120 MPa. The hardening rate quickly decreases, resulting in a plateau-like behavior above shear stresses of 150 MPa and above shear strains of about 0.005.

![Figure 3](image)

**Figure 3:** Shear stress – shear strain curves for a twin double layer with 1000 disconnections in each twin plate. In (a), the grey lines were obtained for initial slope parameters \( p \) larger than 0.2, the black lines for \( p \) smaller than 0.2. While \( p \) smaller than 0.2 results in shear stress – shear strain behaviors where nearly no strain is obtained with up to 150 MPa, lines for \( p \) larger than 0.2 show a significant (for \( p = 1 \) nearly linear) shear strain for an simulated shear stress. (b) shows the two lines with \( p \) very close or equal 0.2. There are large peaks due to a numerical instability originating from weak disconnection-disconnection interaction.

Figure 3b displays results for a slope parameter of approximately 0.2. Large spikes are visible, which are due to numerical instabilities. At a slope parameter of 0.2 the twinning plane inclination angle is 45 degrees. At this angle, there is no disconnection-disconnection interaction force. Small displacements, therefore, have a large effect on the net force on each disconnection. This makes the simulation susceptible to numerical artifacts such as bypass events of disconnections. Bypass events lead to the noise which is particularly large for \( p = 0.2 \) (Figure 3b).

In self-accommodated martensite, the disconnections are located in the hierarchically higher twin boundaries (those containing the disclination walls). For low slope parameters (e.g. \( p < 0.2 \)) the simulations indicate a threshold stress. The threshold stress originates from the
attractive forces between the disconnections, which may be considered as ‘bound’ to the disclination wall. At a large $p$, i.e. when the lateral separation of disconnections is large, disconnection-disconnection interaction is repulsive. The disconnections are detached from the disclination wall. Disconnections can move easily and facilitate twin boundary motion. Thus, the transition of disconnections being bound to the disclination wall to being freely mobile, i.e. the ejection of disconnections from the interface, controls the onset of twinning and, hence, the twinning stress.

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