An Evaluation of a Multi-Scale Material Model Describing Austenite-Martensite Phase Transformation

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Abstract

In this report a newly proposed multi-scale material model for metastable austenitic stainless steels is evaluated. These metastable steels can contain two phases, austenite and martensite. As a consequence of thermo-mechanical loading a phase transformation of austenite to martensite can occur. The phase change is accompanied by a shape- and volume change. Also, the material characteristics of austenite and martensite differ, therefore the material shows a more complex behavior than conventional steel types. On a practical side, these phase transformations can lead to product distortions due to the volume increase and shape change, and thus there is a need for the prediction of material behavior.

The multi-scale material model is aimed at describing the overall deformation behavior while capturing the transformation. Martensite is known to form on 24 crystallographic systems in parent austenite, also called variants. The transformation of one or more of these transformation systems is thought to be the cause of deviating material behavior as opposed to conventional steels. To capture the behavior of an austenite grain, 24 micro-scale models are set up and solved. One micro-scale model captures the behavior of one martensitic transformation system in the austenite and is based of a two layer lamella representing austenite and martensite. Then homogenization is used to average the results towards the overall material behavior of the multi-phase material.

Of special interest in this work is the metastable steel Nanoflex\textsuperscript{TM} of which the properties have already been quantified previously. Experimental observations are used to evaluate the material model. Two important phenomena accompanying mechanical loading of metastable steels are especially important, which are the martensite formation and the TRIP-effect. TRIP (TRansformation Induced Plasticity) is the delay of hardening in the material due to transformation.

To assess the behavior of the material first two single grain orientations, i.e. Goss and copper present in the material, have been modeled in tensile loading. The copper orientation results in less martensite than the Goss orientation. As a consequence, hardening is less than in a Goss grain because less of the stronger martensite phase is present. The difference in behavior between those two single grains is attributed to the activity of the 24 transformation systems. The activation and behavior of transformation systems have been thoroughly examined in this work.

A Representative Volume Element (RVE) consisting of Goss and copper grains is set up to simulate polycrystalline behavior, and is loaded in tension and compression. It can be concluded that the martensite growth is in correspondence with experimental results and is predicted reasonably well by the material model. However, the stress-strain curve of a polycrystalline RVE exhibits an extreme stress-relaxation response at the initiation of transformation, thus significantly deviating from experimental results. Qualitatively, the model behavior is in agreement with experimental material behavior: at the start of transforma-
tion the dilatation and shear strain accommodate the externally prescribed displacement and thereby delay the onset of material hardening (TRIP-effect). Upon increasing the martensite volume fraction the composite hardening effect is observed: the more martensite is present the more the material behavior is dominated by the harder and stronger phase, which corresponds with experimental results. To improve the quantitative predictive power of the model, several suggestions for model enhancement are made in the concluding part of the report.
Chapter 1

Introduction

Advanced steels assisted by the mechanism of transformation-induced plasticity (TRIP-steels) show a good combination of strength, ductility and corrosion resistance in comparison to conventional carbon steels. An example is a TRIP stainless steel Nanoflex™ used in Philips shaver heads, shown in figure 1.1.

The advantageous properties can be traced back to the microstructure in these materials. TRIP-steels contain two phases, austenite and martensite. Austenite is the metastable phase which is able to transform to martensite when subjected to thermo-mechanical loading. It is this transformation that is responsible for the excellent strength-ductility balance exhibited by TRIP-aided steels.

Figure 1.1: Shavercaps and cutters made from Nanoflex™

The irreversible, displacive phase transformation of austenite into martensite is characterized by a crystallographic rearrangement that produces a shear deformation as well as a volumetric expansion. Due to these deformations product distortions are observed on an engineering level. For that reason predictive control is in demand in the form of a material model in conjunction with Finite Element Analysis (FEA).

Different sorts of material models exists: for instance the phenomenologically based macroscale models. These models deal with macroscopic quantities, leading to a description of the
global mechanical behavior only. As TRIP-steels show behavior where the microstructure is responsible for the macroscopic response, it is natural to consider micro-scale models. A microscale model departs from describing the actual physics on a small (micro) level. In conjunction with a multi-scale modeling approach it is possible to describe the macro-scale (engineering) response while still capturing the underlying physics on smaller levels.

In this work the attention is focussed on Nanoflex™ mentioned earlier. Post [13] used a partly physically based macroscopic material model to describe the production process of shaver caps. The model uses a parameter set to quantify the material response for a particular loading case and a specific heat. Slootbeek [15] concluded that this model is unable to correctly predict the mechanical response of tensile and bending tests with one parameter set. In other words, a change in heat or loading requires a different fitted parameter set, which is a drawback. A more generally applicable model is therefore desired.

1.1 Project goal

The present work has been executed as a succession of an article by Kouznetsova and Geers (2008) proposing a multi-scale physically based model. The model is intended for the prediction of structure-property relations for materials exhibiting phase transformations during mechanical loading. The model incorporates the coupling between elastic and plastic deformation of the phases and transformation, the dependance of the transformation on the stress state, the grain orientation with respect to the loading and the history of deformation and transformation.

In this work the model is evaluated for its ability to correctly describe the mechanical behavior of Nanoflex™ both qualitatively and quantitatively. In particular, the capability of the model to capture the TRIP-effect and the S-shape evolution of martensite, which are specific effects seen in mechanical loading of TRIP-steels, is to be evaluated. The available experimental data of this material will serve as an input for the calculations and to confront the model output. Numerical strategies such as the use of Representative Volume Elements (RVE’s) are utilized to model polycrystalline behavior.

1.2 Scope and outline

Grain orientations measured by Orientation Imaging Microscopy (OIM) [8] will serve as input for single and polycrystalline modeling data. To understand the polycrystalline behavior first its building blocks have to be analyzed. Since Goss and copper orientations are frequently present in Nanoflex™ these particular orientations are explored in detail. A description of the experimental observations of TRIP-steels together with a description of the physical background is provided in chapter 2.

The earlier mentioned multi-scale model [6] is based on several micro-scale models consisting of two layers on top of each other. The layers represent the phases austenite and martensite in the material. The multi-scale material model is summarized in chapter 3.

To correctly describe the transformation in the grains a transformation barrier function, earlier proposed [5], is incorporated. As will be explained in section 3.5, transformation is dependent on the plastic deformation of the parent phase (austenite). By adjusting the transformation barrier function a more realistic transformation response can be obtained.
The results of the single grain simulations with orientations Goss and copper are given in chapter 4, where they are loaded with uniaxial tension. The response of the present transformation systems in these grains are given and discussed.

Several sets of different grains are then used in a Representative Volume Elements RVE to model polycrystalline material. The relative positions of Goss and copper grain orientations are swapped and also random orientations are introduced in the RVE. The results will be discussed and explained in chapter 5.

A final discussion follows in chapter 6 where the computational results are discussed. The question is: as to what extent the current state of the model is able to realistically forecast the material behavior. Also, the consequences of certain assumptions in the model are discussed and what effect it has on the model predictions. To improve model predictions several suggestions for model enhancement are made.
Chapter 2

TRIP- Steels

TRIP- steels are a special class of materials: metastable austenitic stainless steels. Metastable steels are in a quasi stable state of equilibrium and contain mainly two phases, austenite and martensite. As a consequence of thermo-mechanical loading, a phase change of austenite to martensite can occur called phase transformation. The phase change is accompanied by a shape- and volume change. Also, the material characteristics of austenite and martensite differ, therefore the material shows a more complex behavior than conventional steel types.

In section 2.1 the physical background is discussed, followed by a summary of some experimental results and observations in section 2.2.

2.1 Physical background

The austenite to martensitic phase transformation is a diffusionless solid state phase change. This means that large number of atoms experience cooperative movements and maintain their relative positions to each other. It is an athermal transformation, the transformation is dependent on transformation temperature rather than the time at that temperature. In steels, martensite is the hardest and strongest (and most brittle) phase that can be obtained in steels.

2.1.1 Thermodynamics

Phase transformations occur when one phase has a lower free energy than the other phase. Free energies of the two considered phases are schematically shown in figure 2.1. Martensite and austenite are in thermodynamic equilibrium at $T_0$. A strong nucleation barrier inhibits the formation of martensite upon cooling the material below $T_0$. Therefore enough energy should be available to overcome this barrier which equals the chemical driving force $U_s$. The amount of chemical driving force needed for the transformation to be solely initiated by temperature difference is found at $M_s$, martensite start temperature, shown in figure 2.1. The chemical driving force is the difference in chemical free energy at $M_s$ between martensite and austenite. At a temperature between $M_s$ and $T_0$ phase transformation does not occur unless assisted by an externally supplied mechanical driving force $U$. The sum of the chemical driving force and the mechanical driving force should equal the chemical driving force at $M_s$, namely $U_s$. This mechanical driving force $U$ can be added by means of mechanical loading. From a physical point of view this is the same as applying stress or strain.
2.1.2 TRansformation Induced Plasticity

TRansformation Induced Plasticity (TRIP) is observed in austenitic meta-stable high strength stainless steels. The TRIP-effect is generally defined as the additional strains by transformation during plastic deformation, resulting in a peculiar stress-strain response. This effect is shown and discussed in section 2.2 on the basis of a tensile test.

Two mechanisms are often considered to explain TRIP-behavior: the Magee [9] and Greenwood Johnson [3] mechanisms. Magee states that a particular variant or transformation system (one or more of the 24 available) is active due to internal stress fields and/or an externally applied stress. The Greenwood-Johnson effect corresponds to the plastic strain in the parent phase as a result of transformation, i.e. martensitic transformation from austenite to martensite triggers plastic straining in the austenite.

2.1.3 Crystallography

Experimental crystallographic observations show that austenite has a FCC (face centered cubic) crystal structure, while the martensite crystal is BCT (body centered tetragonal).

In a continuum sense, transformation is accompanied by a the shear component $\gamma$ and a the dilatational component $\delta$. The latter represents the volume change associated with the phase transformation.

On the assumption of lattice invariant shear, martensite can form on 24 different crystallographic transformation systems [17], also called variants. These variants are fully defined if the atomic spacings of the two lattices or phases are known.
2.2 Experimental results and observations

During forming of TRIP-steels transformation occurs. This leads to product distortions due to the volume increase and shape change accompanied with transformation. Metastable Nanoflex™ is used for corrosion resistant shaver heads. In his thesis Post [13] modeled Nanoflex™ and researched the product distortions of shaver caps due to phase transformations, seen in figure 2.2.

Within Eindhoven University of Technology several experiments have been carried out to qualify and quantify the constitutive behavior of Nanoflex™ [15, 8, 7]. In the following tensile and bending tests, as well as crystallographic characterization are shortly summarized.

![Figure 2.2: Left: Just after stamping. Right: Some time afterwards. Blue is austenite, red martensite. Dimensional change and increase in martensite. Courtesy of Philips DAP.](image)

2.2.1 Tensile test

Structure-property relations have been experimentally quantified for Nanoflex™. Post [13] used inductive sensors to measure the martensitic volume fraction during a tensile test. Similar results [15] have been obtained by an etching procedure [10].

Figure 2.3(a) shows a typical S-shape curve relating the volume fraction of martensite to the tensile strain. There is a typical onset of martensitic formation, where plastic straining of the parent phase (austenite) promotes transformation. Linear growth is seen up to a point of saturation where dislocations formed impedes further transformation [1]. The cause of this phenomenon is further elaborated in section 3.5.

In figure 2.3(b) the stress-strain response is given corresponding to the S-shape martensitic growth. Up until a true strain of 0.03 a conventional response is seen, an elastic part followed by an onset of yielding. Further elongation reveals a plateau ($\varepsilon \approx 0.05$) where ongoing deformation does not result in a significantly higher reaction force. This region is for the left figure (fig. 2.3(a)) dominated by a rise of the martensite fraction. The reaction stress and the growth in martensite are related as a result of the extra strain developed during transformation: transformation strain. The volume and shape change accompanied by transformation accommodates the strain and increases the ductility. This increase in plasticity caused by the martensitic transformation is the macroscopic observation of TRansformation Induced Plasticity (TRIP).

Significant hardening occurs from $\varepsilon = 0.1$, where the relative contribution of transformation strain decreases as less austenite is available to transform and accommodate the deformation. Also, the strength of the formed martensite is playing a more important role in the deformation behavior, this is also called the composite effect. Martensite has a significantly
Figure 2.3: (a) The martensite-strain response of a uniaxial tensile test of Nanoflex™, and (b) the corresponding stress-strain response.

higher yield stress than austenite and as the volume fraction of martensite become sufficiently large, the overall material hardens.

Finally, there is an area in figure 2.3(a) from $\varepsilon = 0.15$ on where the martensitic growth rate stabilizes. Plastic strain in the parent phase impedes transformation as the dislocations hinders further interface movement of the laths. Section 3.5 extends on this subject.

With the aid of upsetting tests characteristics of the separate phases could be singled out (figure 2.4). This data is further on used to estimate the constitutive material behavior of the phases, necessary for the model input.

Figure 2.4: Experimental results of a tensile upsetting test, austenite and martensite. Courtesy of Philips DAP
2.2.2 Bending

Pure bending tests were performed followed by an etching procedure to determine the martensitic content of the metastable Nanoflex™ [15, 7]. A plane-strain state was assumed. Bending is of particular interest where a tensile and a compressive (hydrostatic) stress state interacts with the transformation. In figure 2.5 the amount of martensite is plotted along the thickness of a bend sample. The transformation preferentially occurs in the outer region of the bend. As phase transformation is accompanied by a volume increase, the positive strain (hydrostatic stress) is thought to promote transformation by assisting the volume increase. The negative strain counteracts this volume increase. Because of this obstruction, forming of martensite under compression is delayed. This corresponds to the observations in the literature [12]: $M_s$ temperature is raised by tension and lowered by negative hydrostatic stress.

![Figure 2.5: (a) Picture taken by microscope of cross-section of a bend plate: light gray is austenite, dark is martensite. (b) Martensite fraction as a function of position coordinate $y$. Taken from [7].](image)

2.2.3 Grain orientation observations

Louws [8] investigated the growth of martensite and its dependence on crystallographic orientation of Nanoflex™. With the aid of Orientation Imaging Microscopy (OIM) and optical microscopy he was able to study the microstructure before and after deformation. Mainly Goss and copper orientations were identified in the undeformed sample. The ratio of Goss to copper is estimated as 2:1. A relation between the orientation and the preference of transformation could not yet be detected. Also, X-ray diffraction analysis of the texture of Nanoflex™ yielded similar results [4] concerning the grain orientations.
Chapter 3

Multi-scale material model

3.1 Introduction

Globally speaking, a multi-scale model owns its macroscopic constitutive behavior to the homogenization modeling of the microstructure. In this model [6], the microstructure is modeled and after application of averaging techniques the macroscopic stress, stiffness and martensite fraction are known. Martensite is known to form on 24 crystallographic systems in parent austenite, also called variants. Therefore 24 micro-scale models are set up. One micro-scale model captures the behavior of one martensitic transformation system in the austenite and is constructed of a two layer lamella representing the phases. To capture the behavior of the whole austenite grain, 24 lamellas are solved. Then a homogenization approach will average the results to obtain the complete two-phase material behavior.

The micro-scale model is discussed in section 3.3 after an outline of the multi-scale model is given in section 3.2. Next, homogenization of 24 lamella models is presented in section 3.4. Transformation is highly dependent on the plasticity involved in deformation prior to phase change. This has been verified by several authors and is discussed in section 3.5.

In the following a scalar, a vector, a second- and a fourth order tensor are denoted as \( a, \vec{a}, A, A^4 \), respectively. Cartesian unit vectors are given by \( \vec{e}_i, i = 1, 2, 3 \). An inner product is given by \( A \cdot B = A_{ij}B_{jk}\vec{e}_i\vec{e}_k \), a double inner product by \( A : B = A_{ij}B_{ji} \) and a dyadic product is given by \( \vec{a} \otimes \vec{b} = a_{ij}\vec{e}_i\vec{e}_j \). A transpose of a second order tensor is \( A^T = A_{ij}^T = A_{ji} \).

Jump \([a]\) is defined as the difference of a field quantity across an interface, \([a] = a_A - a_M\) where A and M represent the austenite and martensite respectively. An average of a field is \( \langle a \rangle = \frac{1}{2}(a_A + a_M) \). A complete description of all quantities and operators, as well as all the symbols and abbreviations used in this work is depicted in Appendix A.
3.2 Outline

The outline of the multi-scale model is given in figure 3.1. Three spatial levels can be distinguished, which are connected by in- and outputs. These are the known and unknown quantities \((F_i, P_i, \xi_i, \ i = G, k)\) at every level, illustrated by the bridging arrows. Subscript \(G\) and \(k\) stand for the grain and lamella level, respectively. In the following, a clockwise route along the arrows is followed for elaboration.

In FEA (Finite Element Analysis) the deformation in an integration point is estimated, given by a material point at macro level in figure 3.1. This point belongs to a certain austenitic grain for which the deformation tensor \(F_G\) is imposed. On mesoscale 24 possible transformation systems are reacting to this incoming deformation. This is schematically illustrated by a local deformation tensor \(F_k\) where \(k\) is the specific variant. Current work assumes the Taylor model, where the deformation on every lamella model is equal to the deformation on the austenite grain, i.e. \((F_k = F_G, \ k = 1, ...24)\). Thus, 24 microscale models are subjected to the deformation tensor \(F_G\), whereby each of those models is positioned along a theoretic transformation system orientation. On the right part of figure 3.1 this deformation is now imposed on the lamella model, containing a microscale constitutive model. As a result of solving the deformation of the lamella, equilibrium is obtained between the phases and the stress tensor \(P_k\) and the martensite volume fraction \(\xi_k\) is returned (depicted by the bottom-right arrow). Once all 24 systems are solved, homogenization is executed to determine the systems relative contribution to the whole grain response. The grain stress \(P_G\) and martensitic volume fraction \(\xi_G\) resulting from this step are returned to the integration point level. The constitutive response at macrolevel is now obtained as a result of the incoming stress, together with the material stiffness at the integration point necessary for further iterations.

The orientation relation between the three spatial levels is given by introducing three coordinate systems, as indicated in figure 3.1. These are then interrelated by using orthogonal rotation tensors, mapping vectors of one orientation to the other.

Figure 3.1: Scheme of the multi-scale material model.
3.3 Single transformation system

The micro-scale model is set up by two layers on top of each other. At the start of calculations the microscale model consists of only austenite. Under mechanical loading it can transform into martensite. The interface between the martensite and austenite is referred to as habit plane, depicted in figure 3.2 with its corresponding normal $\vec{N}$. Transformation is accompanied with a shear component $\gamma$ and a dilation component $\delta$. Related to the habit plane the transformation deformation gradient tensor $\mathbf{F}^{tr}$ can be defined, describing the deformation of the martensite as it transforms.

$$\mathbf{F}^{tr} = \mathbf{I} + \vec{M} \otimes \vec{N}$$  \hspace{1cm} (3.1)

With $\vec{N} = [0 \ 0 \ 1]^T$, $\vec{M} = [0 \ \gamma \ \delta]^T$ and $\mathbf{I}$ the second order unit tensor.

![Figure 3.2: Schematic representation of transformation for one lamella.](image)

The martensitic fraction $\xi$ in a lamella is given by:

$$\xi = \frac{V_M^0}{V_0}$$  \hspace{1cm} (3.2)

which is the martensitic volume ($V_M^0$) divided by the total volume ($V_0$) of the lamella.

According to the rule of mixtures the deformation gradient tensor $\mathbf{F}_k$ and the engineering stress $\mathbf{P}_k$ (first Piola-Kirchoff) are distributed between austenite and martensite as follows:

$$\mathbf{F}_k = (1 - \xi)\mathbf{F}_A + \xi\mathbf{F}_M$$ \hspace{1cm} (3.3)

$$\mathbf{P}_k = (1 - \xi)\mathbf{P}_A + \xi\mathbf{P}_M$$ \hspace{1cm} (3.4)

$\mathbf{F}_A$, $\mathbf{F}_M$ and $\mathbf{P}_A$, $\mathbf{P}_M$ are the deformation gradient tensors and the stress tensors of the austenite and the martensite, respectively.

As martensitic transformation is an invariant plane strain deformation, it follows

$$\mathbf{F}_A \cdot (\mathbf{I} - \vec{N} \otimes \vec{N}) = \mathbf{F}_M \cdot (\mathbf{I} - \vec{N} \otimes \vec{N})$$ \hspace{1cm} (3.5)

Stresses these have to be in static equilibrium across the interface which results in the condition:

$$\mathbf{P}_A \cdot \vec{N} = \mathbf{P}_M \cdot \vec{N}$$ \hspace{1cm} (3.6)
Based on the multiplicative split of the deformation gradient of austenite $F_A$ into an elastic $F'_A$ and a plastic part $F^p_A$ it can be written

$$F_A = F'_A \cdot F^p_A \quad (3.7)$$

For martensite, the multiplicative split is different than for the austenite for two reasons: (i) martensite emerges out of the plastically deformed austenite and (ii) it transforms according to the transformation deformation gradient tensor $F^{tr}$. Plastic deformation has occurred in the austenite before it transforms in martensite. This martensite contains more dislocations and is thus harder. This is taken into account by adding the amount of plastic strain of the austenite, prior to transformation, to the plastic strain in the martensite. In other words, the plastic component of the part that transforms is taken over by the plastic flow in the martensite:

$$\varepsilon^p_M = \varepsilon^p_{MM} + \varepsilon^p_A \quad (3.8)$$

where the current equivalent plastic strain of the martensite $\varepsilon^p_M$ is obtained as the sum of the plastic strain of austenite that has undergone transformation $\varepsilon^p_A$ and the plastic strain due to the plastic flow of the martensite, $\varepsilon^p_{MM}$. In tensor form, the plastic deformation of the austenite is incorporated in the multiplicative split of the martensite as $\tilde{F}^p_A$. After transformation, the martensite may deform elastically ($F^e_M$) and plastically ($F^p_M$) to accommodate the deformation on the phases. It is this accommodation together with the transformation ($F^{tr}$) that allows the model to predict the interaction between transformation and plasticity. Taken together, the multiplicative split for the martensite is:

$$F_M = F^e_M \cdot F^p_M \cdot F^{tr} \cdot \tilde{F}^p_A \quad (3.9)$$
3.3.1 Elasto-plastic material model

An isotropic finite strain logarithmic hyper elasto-plastic model \[2\] is used to describe both austenite and martensite, which are in the following indicated by the subscript \(i = A, M\) for the austenite and martensite, respectively. The Kirchoff stress tensor \((\tau_i)\) follows from the elastic left Cauchy-Green (Finger) tensor \(B^e_i = F^e_i \cdot F^{eT}_i\)

\[
\tau_i = \frac{1}{2}^4H_i \cdot \ln B^e_i \quad (3.10)
\]

with \(^4H_i\) the Hookean elasticity tensor

\[
^4H_i = \lambda_i \mathbf{I} + 2\mu_i^s \mathbf{I} \quad (3.11)
\]

The Lamé’s constants are \(\lambda_i = K_i - \frac{2}{3}G_i\) and \(\mu_i = G_i\).

A Von Mises plasticity model with isotropic hardening is considered, where the yield function is

\[
\phi_i(\tau_i, \varepsilon^p_i) = \tau_i^y - \tau_i^y(\varepsilon^p_i) \leq 0 \quad (3.12)
\]

With the equivalent Von Mises stress \(\tau_i^{eq}\) and the current yield stress \(\tau_i^y(\varepsilon^p_i)\).

\[
\tau_i^{eq} = \sqrt{\frac{3}{2}\tau_i^d \cdot \tau_i^d} \quad (3.13)
\]

The current yield stress is obtained by assuming the following exponential hardening law:

\[
\tau_i^y(\varepsilon^p_i) = \tau_i^{y0} + h_i \varepsilon^p_i + (\tau_i^{y\infty} - \tau_i^{y0})(1 - \exp(-\alpha_i\varepsilon^p_i)) \quad (3.14)
\]

with \(\tau_i^{y0}\) the initial yield stress of the phases and \(h_i, \tau_i^{y\infty}, \alpha_i\) being other model parameters.

Energy dissipation in the lamella has three causes: (i) plastic dissipation of austenite, (ii) martensite and (iii) due to the movement of the interface between the two layers. According to the second law of thermodynamics, dissipation rates should be non-negative. The dissipation inequality applied to the lamella leads to a measure of the thermodynamic driving force. This energy is assessed to determine if transformation occurs.

The driving force is given by \[6\]:

\[
G = \langle [\psi] \rangle - \langle P \rangle^T : [F] + P_M^T : \left( F^e_M \cdot F^p_M \cdot F^{tr} \cdot \left( F^p_M - \tilde{F}^p_A \right) \right) - \frac{\partial \psi_M}{\partial \varepsilon^p_M} (\varepsilon^p_M - \tilde{\varepsilon}^p_A) \quad (3.15)
\]

The jump of the chemical free energies between the phases is given by \([\psi]\), by taking into account elastic energy stored and plastic energy dissipated. For the case of purely elastic materials, the first and second terms in (3.15) represent the Eshelby driving force on a discontinuity interface. The last two terms result from the dissipation due to the jump of plastic deformation across the interface and the inheritance of plastic strain in martensite.

Transformation will occur if the driving force \(G\) is larger than a critical value \(G_c\). This approach is similar to elasto-plasticity problems based on a yield surface. Resulting in the equations:

\[
G - G_c \leq 0, \quad \dot{\varepsilon} \geq 0, \quad (G - G_c)\dot{\varepsilon} = 0 \quad (3.16)
\]

The critical value \(G_c\) can be a constant or a function of different variables. In this work it has been chosen for a function dependent on the plastic strain in the parent phase, which will be discussed in detail in section 3.5.
Table 3.1: System of equations.

<table>
<thead>
<tr>
<th>Equation</th>
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<tbody>
<tr>
<td>( \mathbf{F}_k = (1 - \xi) \mathbf{F}_A + \xi \mathbf{F}_M ) (3.17)</td>
</tr>
<tr>
<td>( \mathbf{F}_A \cdot (\mathbf{I} - \vec{N} \otimes \vec{N}) = \mathbf{F}_M \cdot (\mathbf{I} - \vec{N} \otimes \vec{N}) ) (3.18)</td>
</tr>
<tr>
<td>( \mathbf{P}_A \cdot \vec{N} = \mathbf{P}_M \cdot \vec{N} ) (3.19)</td>
</tr>
<tr>
<td>( \mathbf{P}_A = \mathcal{F}_A{\mathbf{F}_A, \varepsilon_A^p} ) (3.20)</td>
</tr>
<tr>
<td>( \mathbf{P}_M = \mathcal{F}_M{\mathbf{F}_M, \varepsilon_M^p} ) (3.21)</td>
</tr>
<tr>
<td>( G - G_c \leq 0, \quad \dot{\xi} \geq 0, \quad (G - G_c)\dot{\xi} = 0 ) (3.22)</td>
</tr>
<tr>
<td>( \mathbf{P}_k = (1 - \xi) \mathbf{P}_A + \xi \mathbf{P}_M ) (3.23)</td>
</tr>
</tbody>
</table>

Until now all the equations concerning one transformation system were presented. To obtain equilibrium of the lamella subjected to the incoming deformation gradient tensor \( \mathbf{F}_k \), a system of equations have to be solved. These seven tensorial equations, as summarized in table 3.1, are all coupled and have to solved simultaneously.

The system consists of averaging relations for the input deformation (3.17) and the resulting stress as output (3.23). Equations (3.18) and (3.19) represent the interface relations, and (3.20) and (3.21) describe the constitutive behavior of austenite and martensite. Finally, the transformation criterion (3.22) is evoked for deciding if transformation occurs.

The system of equations is solved iteratively for the input deformation \( \mathbf{F}_k \). A Newton-Raphson algorithm solves the unknowns \( \mathbf{F}_A, \mathbf{F}_M, \mathbf{P}_A, \mathbf{P}_M \) and \( \xi \). The tangent operator for this system is derived in [6].

Three return maps are active in a coupled fashion. Two of them consist of the elasto-plastic return maps in each phase. The last one is the evaluation of the transformation criterion. If the thermodynamic driving force exceeds the barrier, the whole system of equations is iterated up to the point where \( G = G_c \).
3.4 Homogenization towards grain behavior

Previously, the lamella model for a single transformation system was described. The first step in homogenization is the Taylor assumption \( \mathbf{F}_k = \mathbf{F}_G, \quad k = 1, \ldots, 24 \) where the deformation of the transformation systems equals the grain deformation, as stated earlier in section 3.2. When the lamella model is solved 24 times for all possible transformation systems, a procedure is needed to determine how specific transformation systems account for the total grain response.

A grain is virtually divided in 24 domains, each is represented by a lamella model. One domain represents the collective behavior of all transformation systems whose orientations are equal. One domain thus accounts for all possible martensitic laths arising in the same direction. Hence, the size of the domains is unknown beforehand. It is determined after all 24 systems are solved according to the procedure summarized below.

It is assumed that the volume fraction of one domain \( \eta_k \) is proportional to the volume fraction \( \xi_k \) of martensite that domain produces. A proportionality coefficient \( c \) is taken the same for all systems, thus \( \eta_k = c \xi_k \). As the sum of the domain volume fractions should always equal 1 \( \sum_{k=1}^{24} \eta_k = 1 \), it follows that \( c = 1/ \sum_{k=1}^{24} \xi_k \). The volume fractions of all domains can now be obtained by

\[
\eta_k = \frac{\xi_k}{\sum_{k=1}^{24} \xi_k}, \quad k = 1, \ldots, 24 \tag{3.24}
\]

Consequently, the overall martensitic fraction \( \xi_G \) of the grain is then given by

\[
\xi_G = \sum_{k=1}^{24} \xi_k \eta_k \tag{3.25}
\]

The resulting stresses of lamellas are also taken proportional with the domain size \( \eta_k \), resulting in the average grain stress \( \mathbf{P}_G \)

\[
\mathbf{P}_G = \sum_{k=1}^{24} \eta_k \mathbf{P}_k \tag{3.26}
\]

Note, that with current assumptions, transformation systems producing the most martensite account heaviest in the total grain behavior. When, for instance, 2 out of 24 systems produce martensite, the grain response is assumed to be totally defined by these 2 active systems. Consequently, inactive systems are assumed to play no roll in the constitutive behavior of a deforming and transforming grain.
3.5 Plasticity dependent transformation

It is known in the literature [11] that by plastic straining of the austenite, martensite nucleation sites are formed, which enhances the formation of martensite. A commonly observed nucleation site is at shear band intersections, where the pile-up of dislocations results in crystal faults and internal stresses and thus promotes transformation [16]. These experimental observations have been recently revisited by molecular dynamics (MD) calculations. The shear band intersections proved to provide sufficient conditions for transformation [14].

On the other hand, the presence of dislocations is also thought to be the cause of a gradually stagnating transformation. Chatterjee et al. [1] found that an increase in dislocations will prevent the martensitic volume fraction in the sample from growing towards 1. Dislocations surround the laths and prevent possible interface movement. This is measured on the macro-scale as a stabilization zone where ongoing strain does not result in more martensite (right of S-shape curve fig. 2.3, sec. 2.2).

In the model, calculations require that the thermodynamic driving force in austenite should reach or exceed the transformation barrier \( G \geq G_c \) to initiate transformation. For that reason, choosing the transformation barrier dependent on the plastic strain in the parent phase was proposed [5]. In the following we consider a piecewise-linear function \( G_c(\varepsilon_{PA}) \), as given in figure 3.3, where the critical driving force \( G_c \) is dependent on the amount of plastic strain in the austenite \( \varepsilon_{PA} \). A horizontal start indicates that not enough dislocations are yet piled up to create additional nucleation sites. The initial level of \( G_c \) corresponds to the transformation barrier on cooling. This changes as plastic strain continues in the austenite, leading to an increase of the martensite nucleation sites. This is modeled by a drop in the transformation barrier \( G_c \). Finally, a rise in the barrier indicates dislocations pile-up for larger strains in the parent phase, suppressing further transformation.

![Proposed transformation barrier function dependent on the plastic strain in the parent phase.](image)

Figure 3.3: Proposed transformation barrier function dependent on the plastic strain in the parent phase.
Chapter 4

Single grain simulations

4.1 Introduction

As we are interested in the prediction of mechanical behavior on macro-level, we incorporate the experimental observed characteristics of our material of interest. As explained in chapter 2.2 the dominant grain orientations in the as-received Nanoflex\textsuperscript{TM} are Goss and copper. It would be natural to assign these orientations to our Representative Volume Element (RVE). Before making any conclusions about the response at macrolevel of an RVE, the single elements are explored in detail in the upcoming paragraphs. To fully understand the behavior of a mixture of elements, it’s building blocks, single grains, should be analyzed thoroughly first. After the different (elasto-plastic) input parameters are presented, the computational results are given and discussed in this chapter.

4.2 Model input

One 8-node brick element has been subjected to uniaxial tensile stress. Grain orientations of Goss and copper are adopted for these elements. The elasto-plastic input parameters are given in table 4.1, fitted to resemble characteristics of the single phases given in chapter 2.2.

Applying these input parameters to the material model result in the tensile test responses of the individual phases given in figure 4.1. The shear and dilatation component are $\gamma =0.226$

![Figure 4.1: Model tensile test responses of individual phases austenite and martensite](image)
Table 4.1: Material parameters of austenite and martensite.

<table>
<thead>
<tr>
<th>Phase</th>
<th>$E$ (GPa)</th>
<th>$\mu$ [-]</th>
<th>$\tau^y_0$ (GPa)</th>
<th>$\tau^y_\infty$ (GPa)</th>
<th>$h$ (GPa)</th>
<th>$\alpha$ [-]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Austenite</td>
<td>210</td>
<td>0.3</td>
<td>0.353</td>
<td>0.686</td>
<td>0.561</td>
<td>11.2</td>
</tr>
<tr>
<td>Martensite</td>
<td>210</td>
<td>0.3</td>
<td>0.814</td>
<td>1.055</td>
<td>0.1</td>
<td>26.1</td>
</tr>
</tbody>
</table>

and $\delta = 0.0213$, respectively.

Transformation occurs when the thermodynamic driving force exceeds transformation barrier. An optimization procedure is executed to let the formation of martensite resemble the experimental results and the obtained transformation barrier function is depicted in figure 4.2.

Figure 4.2: Proposed transformation barrier function dependent on the plastic strain in the parent phase.
4.3 Results

4.3.1 Tension

In figure 4.3 the stress strain responses are given of grains with Goss and copper orientation. The true stress in the loading direction plotted against the true strain yields quite different results for the two orientations. Note that this material behavior of different grains does not have to represent experimental results since experimentally attaining the response of single grains in this material is not (yet) feasible.

![Graphs showing stress-strain responses for Goss and copper orientations.](image)

Figure 4.3: Uniaxial tests of one element Goss and copper.

The left graph (figure 4.3 (a)) shows that up to 6% strain the responses of Goss and copper are identical. Ongoing strain until 8% produces a drop in the uniaxial stress. This drop is for Goss more apparent than it is for copper. For copper the reaction force has only a slight drop, followed by a gradual increase. This is also the case for Goss, however, the drop in reaction stress is larger as well as the hardening behavior starting from $\varepsilon = 0.16$ for Goss.

This behavior can be traced back to the formation of martensite given in the figure 4.3 (b). The martensitic fraction is plotted versus the true strain. No martensite is formed up to the aforementioned point of 6% strain. Martensitic growth in the Goss grain starts somewhat earlier. This can be seen back in the stress behavior. The formation of martensite is accompanied with a volume increase and a shape change. This clearly relaxes the material response. Copper shows similar relaxation behavior after more straining, however significantly less. The rate of martensitic formation is almost half of that of Goss while the relaxation is not in proportion with that observation. This implies that another effect is present as well, possible by the specific variants that are active, which is dealt later on.

As the martensite volume fraction increases (and reaches 1 at about 21% strain for the Goss grain, figure 4.3 (b)), the accompanying stress-strain response is gradually reflecting the stress-strain model response of martensite given in section 4.2. As more volume fraction of the grain consists of martensite, it’s overall behavior will show the response of the product phase which is called the composite effect. The extra hardening as a result of transformation is referred to as transformation hardening. And as the martensitic fraction in the Goss crystal is larger than in copper, transformation hardening is more pronounced in a Goss element.

The transformation barrier, earlier given in figure 4.2, starts relatively high with a sharp drop after the plastic straining in austenite reaches $\varepsilon^p_A = 0.055$. This drop coincides with
the formation of martensite, since both Goss and copper are reacting to this decrease in the transformation barrier by forming martensite. Continuing straining results finally in an increase of the transformation barrier which inhibits transformation however in present tensile test this point is not reached, which will be verified later on.

In figure 4.4 the deformed 8-node elements of both grains are given (3 × magnified). The copper grain shows a different deformation, as shear is observed. In later chapters this will be elaborated.

Figure 4.4: Element after 30% strain for Goss (top) and copper (bottom). 3 × magnified. From left to right: 3D-, front- and side view.
4.3.2 Goss grain

Since the elasto-plastic behavior of the single phases in every transformation system is the same in current framework, the difference of total grain response is only dependent on the variant selection. Therefore a closer look is taken at specific variants, i.e. under what circumstances they become active and transform.

Transformation occurs when the driving force acting on a variant reaches the critical value (here the transformation barrier $G_c$). The most favorably oriented variants reach this critical value earlier. According to the theory of Wechsler et al. [17] the orientation of 24 possible crystallographic transformation systems are known in the parent phase (austenite). Thus the orientation of all transformation systems are known for the grains of interest, i.e. Goss and copper. In figure 4.5(a) the normals ($\vec{N}$) of all variants of Goss are given in 001 pole figures. The right figure 4.5(b) shows normals of active systems as they form martensite during straining.

In total 16 transformation systems are active, representing two different angles with respect to the tensile direction ($x$-axis). Figure 4.6 shows the martensite fraction produced by the transforming variants. The normals of the variants which produce the most martensite make an angle of 39.3 degrees with the loading axis (variants 17-24, see fig 4.6). The less transforming variants (5-8, 13-16) are located at 79.7 degrees from the $x$-axis. The remaining 8 systems (1-4, 9-12) are inactive making an angle of 52.6 degrees with the loading direction.

Figure 4.5: 001 pole figures of Goss orientation: (a) all possible variants and (b) active variants in uniaxial ($x$-direction) loading. Legend: Angle of transformation system w.r.t. the loading axis ($x$-axis), and number of system.

The theory of Patel and Cohen [12] suggests that the work done by transformation is added to the thermodynamic driving force. They have derived the work done by transformation as given in equation (4.1). Therefore, on certain angles with respect to the loading axis, transformation occurs preferentially if the stress direction is in the direction of transformation (in direction of shear and dilatation). For the values of $\gamma$ and $\delta$ used, the most favorable transformation system is oriented at 42.3 degrees with respect to the loading axis according to the following equation,

$$\frac{U}{\sigma} = \frac{1}{2} \gamma \sin 2\theta \pm \frac{1}{2} \delta (1 + \cos 2\theta)$$

(4.1)
The $\sigma$ is the uniaxial stress, $\gamma$ and $\delta$ are the shear and dilatation components, respectively. The angle between the normal of the variant and the tensile direction is given by $\theta$. The work by transformation $[U]$ normalized by the stress $\sigma$ is plotted in figure 4.7.

Indeed the variants with normals oriented closest to the most favorable direction produce the most martensite (fig 4.6). These variants (17-24) make an angle of 39.3 degrees with the tensile axis. Variants 5-8 and 13-16 also produce martensite, but are oriented at 79.7 degrees with loading axis. An angle of 52.6 degrees with the loading axis (variants 1-4, 9-12) seems not to induce enough transformation driving force for transformation. Although it should be more favorable according to figure 4.7 than the angle of 79.7 degrees. However, the theory of Patel and Cohen is restricted since it does not take into account the moving interface as well as the interaction between transformation and plasticity.

Transformation can then be explained by paying attention to what causes transformation. In chapter 3 it has already been mentioned that transformation occurs if the transformation driving force exceeds the transformation barrier. The driving force (normalized by the initial
critical driving force $G_c^0$ used in the present model is given by:

$$\frac{G}{G_c^0} = \left( \left[ \psi \right] - \langle \mathbf{P} \rangle^T : \left[ \mathbf{F} \right] + \mathbf{F}_M^e : \mathbf{F}_M^p : \mathbf{F}^{\text{tr}} \cdot \left( \mathbf{F}_A - \tilde{\mathbf{F}}_A^p \right) \right) / G_c^0$$

$$- \frac{\partial \psi_M}{\partial \varepsilon_p} \left( \varepsilon_A^p - \tilde{\varepsilon}_A^p \right) / G_c^0$$

(4.2)

The first and second terms in equation (4.2) represent the driving force on a discontinuity interface, known as the Eshelby driving force for elastic materials. The last two terms give the dissipation due to the jump of plastic deformation across the interface. The difference between the first two terms for each set of martensite variants is plotted in figure 4.8. It shows the difference of the chemical energies between the phases and the influence of the stress state across the interface. The results are in correspondence with the martensitic transformation of these variant groups, i.e. the Eshelby driving force before the start of the transformation (up to approx. 6% strain) is simply the largest for the most active variants, followed by the second group of the transforming variants. Therefore the main contributor to the variant selection is the influence of the stress state across the interface. Transformation initiation at about 6% strain causes the Eshelby driving force to drop due to a relaxation which can be seen in the global stress-strain response figure 4.3 (a). Variants 5-8 and 13-16 exhibit a strong downward trend after 6%, as we will see later on it is due to a large plasticity component which lowers the elastic contribution.

In figure 4.9(a) the plastic strain in the austenite (a) ($\varepsilon_A$) and in the martensite (b) ($\varepsilon_M$) is shown for every variant. In the austenite it is seen that up to a point of 6% strain the plastic strain in every variant is the same. After that point transformation starts and interaction between the phases causes the plastic strains to diverge. Logically, in the martensite (fig. 4.9(b)) there is no plastic strain up until the initiation of martensite. In both the figures it is seen that the most active systems (17-24) have undergone the least amount of plastic deformation in both the austenite and the martensite. This indicates that transformation complies with the deformation when variants are preferentially located. In the austenite (fig 4.9(a)) a vanishing
point exist at $\varepsilon = 0.15$ because these variants are 100% martensite from that point on. The plasticity evolution in the martensite corresponds with that observation (fig 4.9(b)). After the transformation is finished, the applied straining cannot be accommodated by martensite formation, thus resulting in the increased plastic deformation rate.

For the slower transforming systems (5-8, 13-16) the plastic strains are the highest. These variants are positioned in such a way that to accommodate transformation, austenite has to deform plastically at an increasing rate. The remaining variants 1-4, 9-12 are not active, thus plastically deform linear in the austenite due to the absence of interaction with martensite.

Figure 4.9: Plastic strain in the parent phase (a) and the product phase (b) of every variant.

The total deformation tensor of a Goss grain is given in equation (4.3).

$$
\mathbf{F}_{\text{Grain}} = 1.3 \hat{\varepsilon}_1\hat{\varepsilon}_1 + 0.886 \hat{\varepsilon}_2\hat{\varepsilon}_2 + 0.886 \hat{\varepsilon}_3\hat{\varepsilon}_3
$$

(4.3)

Note that the determinant is of the $\mathbf{F}_{\text{Grain}} = 1.02$. This 2% volume increase is the result of the $\delta$-component inherent in transformation.
4.3.3 Copper grain

Figure 4.10(a) shows all the variants of a copper oriented grain. Uniaxially loading this grain activates all the possible systems where every variant is forming martensite to some degree (figure 4.10(b)). From the 001 pole figure one can see that the variants are not positioned symmetrically with respect to the loading direction, like in the case of Goss orientation. The angles between the tensile direction (x-axis) and the variants can be divided into four groups of 6 variants each (25, 46, 78 and 89 ± 1 degrees).

Virtually similarly positioned variants produce quite different martensitic fractions. However, this tensile test is hardly comparable to the deformation of the previous case. This is seen in the following equation

\[
\mathbf{F}_{\text{Grain}} = 1.3 \hat{e}_1 \hat{e}_1 - 0.012 \hat{e}_1 \hat{e}_2 - 0.017 \hat{e}_1 \hat{e}_3 + 0.889 \hat{e}_2 \hat{e}_2 + 0.008 \hat{e}_3 \hat{e}_2 + 0.878 \hat{e}_3 \hat{e}_3 \quad (4.4)
\]

where the deformation gradient tensor of the whole grain is given. Three shear components are introduced as opposed to a standard tensile experiment. Note that also the transverse contractions with respect to the tensile direction are not equal (\(\hat{e}_2 \hat{e}_2 \neq \hat{e}_3 \hat{e}_3\)). The cause of this distortion of a cubic element can be traced back to the nonsymmetric positioned variants. When particular variants are active, a volume increase and shape change occurs. If the active variants are not located symmetrically with respect to the tensile direction, these geometric changes of the variants will result in a rectangular prism. Whereas a conventional material forms a square prism as a result of uniaxial tension. The volume increase of this element (\(\det(\mathbf{F}_{\text{Grain}})\)) is 1.5%, which is lower than the dilatation component \(\delta (=0.0213)\). The martensite fraction of the this copper grain is almost 60% at this point, and therefore not all dilatation has occurred.

Since the Taylor approach is assumed at the level of transformation systems, the same deformation is imposed on every variant. The scatter in the results of similarly positioned variants is probably due to the shear components present and the unequal transverse contractions. The shear strain sometimes aids and in some cases hinders transformation depending on the shape deformation vector. This also results in the fact that transformation system making a 79° ± 1° angle with the loading direction produce more martensite than all the
others. While in the Goss grain the variants located at 39.3° are more active than the ones located at 79.7°.

Reconsider the stress-strain curve (fig. 4.3) for copper introduced in the beginning of this section. The relaxation of the reaction stress at the instance of transformation was much less for copper orientation than for Goss. One possible reason, mentioned before, was that the martensitic growth rate is less. Also the activation of all (unsymmetrically placed) variants could be a reason. The reaction stress is simply the result of many active systems that transform in all possible directions, thereby ‘dampens’ the effect of a macroscopic stress reduction.

The difference between variants is also observed when the plastic strain of austenite and martensite are plotted (fig 4.11).

![Figure 4.11](image)

Figure 4.11: Plastic strain of variants in austenite (a) and in martensite (b) for a copper grain.

Interestingly, the difference between plastic strains of the variants located at 78- and 89 degrees is minimal. Transformation systems located at 25 and 46 degrees have a larger scatter of the strains, i.e. the difference of plastic strains of mutually located variants is larger. The more a variant lies along the favorable orientation (42.3°), the more susceptible plastic strains are for shear components in the overall grain deformation.

Previous calculations were done with 8-node brick elements, which are limited to a constant strain state within each element. Therefore the grains behavior is forced to comply with a homogeneous strain state. In order to verify if it is correct to assume one 8-node element to describe one grain, a test is done where a grain is divided into more elements. This allows the strain and stress vary within the grain. If static equilibrium is established through varying strain field through the elements, then more elements are necessary are describe these single orientations. This is not the case as can be seen in Appendix B, where homogeneity of all elements with the same orientation is observed. Therefore one element gives equal stress strain behavior as multiple elements.
Chapter 5

Polycrystalline simulations

5.1 Introduction

In the previous chapter, the transformation and deformation behaviors of single grains of two particular orientations have been scrutinized. The real material, however, consists of a large collection of single crystals interacting with each other in different ways. In order to explore the transformation and deformation behavior of polycrystalline samples, in this chapter several Representative Volume Elements (RVE) reflecting different textures have been set up.

The uniaxial tensile tests on three RVE’s are used to investigate the influence of particular texture on the overall transformation behavior and stress response of the material, as well as on the local stress and strain fields that develop with the grains.

Next, a uniaxial compression test of one RVE is conducted and the transformation and stress response is compared to a tensile test.

5.2 Model setup

To simulate polycrystalline material several Representative Volume Elements (RVE), each consisting of 27 single crystals, have been set up. This choice of the number of crystals modeled allowed to reasonably represent the textures of interest, while keeping the computation time at minimum.

Three simulated sets of grain orientations are given in table 5.2. The first set called “Nano” reflects the preferential Goss and copper texture components in the ratio 2:1. To simulate the slight deviation of real crystal orientations from these idealized textures, a random distribution of 5 degrees has been imposed on the Euler angles. The effect of this can be seen in the 001 pole figures in table 5.2. To investigate the effect of the placement of grains within the RVE, the position of Goss and copper oriented grains have randomly been interchanged three times, resulting in three variations of the “Nano” orientation set, as shown in figure 5.1, and in the following named: “Nano 1”, “Nano 2” and “Nano 3”.

Another set of orientations, termed “Mix” consists of 2/3 Goss and copper grains taken in the proportion 2:1, supplemented by 1/3 of randomly oriented grains, see table 5.2. Finally, one set of completely randomly oriented grains has been generated and is called “Random”.

The input parameters of the transformation model are the same as described before in section 4.2. To reduce the computation time only one finite element per grain is used. All
<table>
<thead>
<tr>
<th>Set</th>
<th>Name</th>
<th>Grains</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Nano</td>
<td>18 Goss + 9 copper</td>
</tr>
<tr>
<td>2</td>
<td>Mix</td>
<td>12 Goss + 6 copper +9 random orientations</td>
</tr>
<tr>
<td>3</td>
<td>Random</td>
<td>27 random orientations</td>
</tr>
</tbody>
</table>

Table 5.1: Grain orientation sets consisting of different grains, used as input in RVE simulations.
Figure 5.1: Different positions of Goss and copper orientation in RVE. Yellow is Goss and red is copper. From left to right: Nano 1, Nano 2 and Nano 3. Tensile direction is $\vec{e}_1$.

RVE’s are loaded in uniaxial tension in the rolling direction using the procedure involving the periodic boundary conditions, as described in Appendix E.
5.3 Results

5.3.1 Tension

The results of uniaxial loading of the five grain orientation sets are given in figure 5.2. In figure 5.2 (a) the corresponding martensite evolutions are presented. The amount of martensite shown is the average of all 27 elements. Just like in chapter 4, the drop in stress at 6% strain is related to the start of martensitic transformation at about the same strain. The growth in martensitic volume fraction is also here related to the drop in reaction stress. After about $\varepsilon=0.15$ the growth of martensite slows down. This is caused by variants in Goss grains that reach a martensitic volume fraction of 1. The result is that the overall grain show less martensite growth. Also, upon reaching this fraction, hardening is observed in the stress-strain curve at $\varepsilon=0.15$ which is a direct result of saturation of some variants. This shown and discussed later on in this section. The RVE’s containing random orientations produce different results from the Nano sets. The upward trend of martensite is somewhat smaller. The curve stops around $\varepsilon=0.15$, hence, it is unclear if a stagnation of martensitic growth is present there.

![Figure 5.2: (a) Martensite growth-true strain (average over whole RVE) and (b) true stress-strain curves of the five orientations.](image)

The stress-strain curves in figure 5.2 (b) show similar behavior until a strain of 6%. Then a drop in stress occurs, followed by two regions where hardening occurs. For “Nano” 1, 2 and 3 a mild hardening region from $\varepsilon=0.8$ until $\varepsilon=0.15$ is followed by stronger hardening from $\varepsilon=0.15$ on. These three sets “Nano 1”, “Nano 2” and “Nano 3” produce almost equal stress response. The observed drop in stress is the largest for the sets of “Nano” orientations. The mixed case, where Goss and copper are mixed with 1/3 random angles, show a moderate drop. If the RVE consists of completely randomly oriented grains this drop is even less.

In figure 5.3 the polycrystal response obtained from one of the “Nano” sets is plotted together with the single grain responses from chapter 4. The “2:1 averaging” means that the single grain responses are weighted to equal their fractions in the polycrystal “Nano”. The result largely coincides with the polycrystal response. There is however a slight deviation in the region where martensite growth is the largest. The difference could be caused by: interaction between the grains, the variation of Euler angles in the polycrystal or the fact that the natural tendency of shearing for copper is obstructed.

The macroscopic RVE’s stress proved to be the same for all “Nano” cases (see Fig. 5.2), i.e.
Figure 5.3: (a) Stress-strain curves of the polycrystal “Nano” compared to the single grain responses of Goss and copper, and (b) the corresponding martensite growth. “2:1 Averaging” is the summation of 1/3 of single copper element response with 2/3 single Goss element response.

regardless of the position of the Goss and copper grains. The connectivity of the phases have no consequence for these calculations. Note that this does not mean that the RVE exhibits isotropic material behavior, these specific orientations are only valid when displacement occurs in the rolling direction. A tensile strain perpendicular to the rolling direction could induce other material behavior since different transformation systems become more preferable.

The equivalent Cauchy stresses are depicted in figure 5.4. At a true strain of 18%, three Nanoflex RVE’s show roughly equal equivalent Cauchy stresses, only at different positions. Mainly two colors can be identified: orange at ≈ 930 MPa and blue at ≈ 730 MPa. The stresses of Goss orientations (orange) indicate the highest values, and the copper orientations (blue) reflect the lowest. The Goss orientation contribute a greater extend to the load bearing of the RVE, this is due to a larger martensite volume fraction in the Goss grains. The specific Cauchy stresses corresponds well with the single grain stresses given in the previous figure (Fig. 5.3). The position of Goss and copper grains does not influence equivalent internal stress fields.

Note that the stress distribution in the RVE given in figure 5.4 is opposite at 7 - 15% strain where the Goss phases exhibit relaxation due to transformation, which is depicted in figure 5.5. At 10% applied strain the strongest grains are the copper grains which show the least reaction stress at 18% given previously in figure 5.4.

The RVE orientation sets “Mix” and especially “Random” show a characteristic difference compared to the internal stress fields of the “Nano” sets. In figure 5.6 the equivalent Cauchy stress fields are given at 10% applied strain. The “Mix” RVE contains Goss and copper orientations which show comparable stresses as given earlier in figure 5.5 for the ”Nano” sets, added with random grains. The ”Random” grain orientation set show a more homogeneous internal stress field. Most grains are depicted by a yellow color accompanying a stress of about 550 [MPa] at 10% strain. This stress coincides with the reaction stress of a copper grain in a “Nano” calculation, which is related to the activation of the amount of transformation systems in a grain. Basically, only Goss-like orientations show a large drop in stress whereas other oriented grains (“Random”, Fig. 5.6) show relatively similar stresses.
The “Nano” calculations can be thought of as a composite containing hard and soft components with relatively high volume fractions (Goss 67% and copper 33%). At 18% strain the hard micro-phases are the Goss and the soft phases are copper orientation. In figure 5.7 the equivalent strain is plotted, where it is seen that strains are in close range, between $\varepsilon_{eq} = 0.195 - 0.2$. One can say that a homogeneous strain situation is present without imposing such a condition. An interesting observation regarding the local strains can still be made. Areas where more copper grains are present (page 32, fig. 5.4 blue elements), result in a somewhat smaller equivalent strain, seen in figure 5.7. This is a contradictive observation because the copper grains are the softer phases and should result in a larger
Figure 5.6: Equivalent Cauchy stress [GPa] of the RVE’s internally. Taken at 10% applied true strain. Left is “Mix” and right is “Random”. Tensile direction is \( \vec{e}_1 \)

equivalent strain, since the load bearing capacity is smaller. A composite matrix material can be larger strained if more softer phases are contributing. The answer can be found in the volume increase caused by transformation. As stated in chapter 4, the fast transforming Goss grains result in more dilatation strain than their counterparts of copper. So the result is that, although Goss is stronger, it also has more volume increase which in turn results in more equivalent strain. The effect is that the strongest phase in the composite contributes more strain in the RVE than the softer phase.

As stated earlier in the model input, section 5.2, certain random distributions around Goss and copper orientations are used in the simulations. By slightly altering the orientation of a grain, other variants could become more favorable and active. In figure 5.8 the martensitic responses of all possible variants of 18 grains of Goss are shown, illustrated with an average and a spread. The average reaction of the variants of 18 Goss grains (fig. 5.8) is again divided in three groups of variants, as done earlier in chapter 4.

It can be seen that a variation of five degrees is enough rotation to induce variants to become more favorable than others within the same group, depicted by a spread. However, this deviation is entirely within the groups. The same active groups show largely equal activity as in uniaxial tensile loading of a single Goss grain. The RVE calculation deviates in two ways from single grain simulations: (i) a different stress field due to the mixture with copper grains and (ii) a variation of 5 degrees of their orientation. This is however not sufficient to induce a completely different transformation behavior of the variant groups, e.g. it does not result in a driving force sufficient to induce transformation in the idle 5-8 and 13-16 variant
Figure 5.7: Total equivalent strain inside the RVE’s. Taken at 18% true strain. From left to right: Nano 1, Nano 2 and Nano 3. Tensile direction is $\vec{e}_1$.

Figure 5.8: Martensite fraction per variant versus applied true strain, average of 18 Goss grains in “Nano 1” orientation set. Divided over three groups of variants.

As has been mentioned, the drop in reaction stress is less for RVE’s with more randomly oriented grains. The “Mix” RVE contains 9 random oriented grains and the “Random” RVE 27. Goss orientation typically activates 16 variants, whereas copper and most random grains activates almost all variants. In chapter 4 it was already mentioned that a single grain of copper shows a small drop in stress upon transformation due to the fact that all variants, differently oriented with respect to the loading direction, are active. On a larger scale (RVE) this is seen again, as shown in figure 5.9. The more variants produce martensite, the less is the drop in reaction stress during martensite transformation as schematically indicated in...
Figure 5.9 (a). The absolute difference is however not that large, suggesting that other causes

could also be present. A random orientation results in randomly oriented transformation systems. If randomly transformation systems are forming martensite, dilatation and shear occur in a random fashion. It looks like the more random transformation is present, the less of a stress-relaxation phenomena is present. On the other hand, the “Nano 1,2,3” with 18 Goss orientations show a profound drop in stress due to the symmetrically oriented transformation systems seen in single grain simulations, regardless of 5 degrees random variation on idealized orientations. Another cause is the martensite evolution seen in figure 5.2 (a), random grains in an RVE result in somewhat less overall martensite possibly leading to a smaller drop in reaction stress.

Figure 5.9: Number of active variants for RVE with 27 elements (a), and the corresponding true stress-strain responses (b).
5.3.2 Compression

The results of the compressive uniaxial loading of 27 elements have been compared to the uniaxial tensile results, see figure 5.10. Obviously, the results prior to transformation are the same. After the onset of transformation, a relaxation of the RVE reaction stress occurs, but less than in tension. Different variant behavior could be the reason for this smaller drop which will be discussed in a following paragraph. The computational results are in qualitative agreement with experimental result, as it has been proven that compression also induces transformation [12] but less than in tension. Also, bending experiments show significantly less martensite in the compressive part of a bend, as given in section 2.2. Note, the difference between tension and compression given here is not that large possibly due to a different stress state, uniaxial compression as opposed to a plane strain condition in bending of a plate.

Although the TRIP-effect has also been observed in compression and is modeled here in a qualitative way, such a large drop in stress seems somewhat counter-intuitive. Suddenly compression seems to go easier once transformation is started, which is somewhat hard to imagine. This is however an inherent part in the material model. A grain stress behavior is the summation of the reaction stresses of transforming variants. Due to the fact that differently positioned variants produce martensite, the stresses in the compression direction of active variants can vary and causing somewhat unexpected responses of a crystal in the loading direction.

![Figure 5.10: (a) True stress-strain curves of the Nano orientation set (27 elements), compression versus tension, (b) corresponding martensite growth (average over whole RVE).](image)

The figure 5.11 shows the averaged martensitic contents of 18 Goss elements in a polycrystal of the “Nano” orientation set in uniaxial compression. The spread of the martensitic response, due to a angle variation of 5% of the angles, is omitted for clarity. Compression typically actives all variants available, perhaps one of the reasons the drop in reaction stress is less than in tension. The most active variants in compression are 5-8 and 13-16 and have habit plane normals with 79.7 degrees from the compression x-axis. In tension these variants were the second fastest transforming indicating orientation (Magee) effect has taken place. The variants 1-4 and 9-12 are the second active group making an angle of 52.6 degrees with the loading direction, which were in tension completely inactive. The least transforming variants 17-24 (39.3 degrees) are slightly active as opposed to tension case where this group produced...
maximum transformation.

When applying equation (4.1) from [12] to compression it appears that for the chosen material parameters a habit plane with 48 degrees angle with the loading direction is the most favorable. This angle is closest to the group variants 1-4 and 9-12 which is activated, however only second in martensite production. Similar observations are earlier noticed in tensile experiments in section 4.3.2: the orientation of the normal ($\mathbf{N}$) with respect to the loading axis is important but not the determining factor. This is the result of the nature of the criterion of Patel and Cohen [12] since it is only dependent on orientation and externally applied stress, while in the current model plasticity influences transformation behavior to a great extent. The intrinsic interaction between transformation and plasticity in a variant sometimes overrules the compliance of the transformation strain with the external stress. This is indicated by the fact that 5-8 and 13-16 variants should be the most active, but are overtaken by variants that have habit plane normals making 79.7 degrees angle with the loading axis.

![Graph]

Figure 5.11: Martensite-true strain, average of 18 Goss grains grains in compression. Divided over three groups of variants.

Finally, a calculation is executed to verify whether 27 grain orientations is representative for the polycrystalline material model response. An RVE consisting of 216 randomly oriented grains loaded in uniaxial tension and compared to the result of the “Random” grain orientation set of 27 grains used in this chapter. The difference proved to be very little which can be seen in Appendix C.
Chapter 6

Conclusions and recommendations

6.1 Conclusions

To evaluate the behavior of the implemented material model single grain orientations Goss and copper have been loaded in uniaxial tension. These orientations are the main crystal orientations observed in the material Nanoflex\textsuperscript{TM} [4]. Next, a polycrystal containing the before mentioned orientations have been loaded in tension and compression. The material model predictions have been found to be in qualitative agreement with experimental results, it is however quantitatively deviating from experiments. In the following paragraphs the computational findings are briefly summarized.

6.1.1 Single grain simulations

A single grain of Goss orientation follows the elasto-plastic behavior of pure austenite up to approximately 6\% strain. After that, a drop in reaction stress is observed followed by a gradual increase and later after about 15\% strain a significant increase in stress. The drop is related to the initiation of transformation which is accompanied with an increase in volume and a shear component in the variants, and the increase in stress after 15\% strain is caused by a saturation of the active variants. A saturation of variants occurs when, due to transformation, they become completely martensitic and lead to a higher reaction stress. The initial drop in stress at 6\% has been found to be linked to the form of the transformation barrier function chosen as model input. Increasing plastic strain in the austenite results in an effectively lower barrier, i.e. at a certain strain the likelihood of transformation is increased. The shape of the transformation barrier function is phenomenologically based on physical observation: since plastic strain in the parent phase initiates additional nucleation sites for transformation [11, 16, 14], transformation probability is increased.

It has been shown that the transformation variants in a Goss grain are positioned in a symmetric fashion with respect to the tensile direction and can be divided in three groups (each contains eight variants) with the normal of the habit plane making a specific angle with the loading direction: 39, 53 and 80 degrees. In tension, variants with normals making a 39 degree angle with the loading direction proved to induce the most martensite. This is in accordance with the theory of Patel and Cohen [12] which states that the work done by transformation can be added to the chemical driving force for the transformation. However, an angle of 53 degrees results in no transformation at all, while variants making an angle of 80 degrees do transform. According to the before mentioned theory this should be the other
way around. The theory of Patel and Cohen, however only incorporates an externally applied stress and the orientation of transformation. The current material model incorporates also the intrinsic interaction between the transformation and plasticity which results in different material response activating different variants.

One grain of copper orientation shows less transformation. As a consequence, the composite hardening is less than in a Goss grain. The drop in stress is also less than in the Goss grain, which is explained with variant behavior. The copper orientation typically initiates (almost) all variants present. Due to the activity of all (non-symmetrically positioned) variants the stress relaxation is smeared out, and thus the drop in reaction stress upon transformation is significantly smaller. Also, the overall resulting grain deformation behavior under uniaxial tension shows three non-zero shear components due to the uneven activity of these non-symmetrically positioned variants. The transverse contraction strain in the directions perpendicular to the loading direction are also unequal as a result of this.

6.1.2 Polycrystalline grain simulations

To investigate the influence of the grain interaction, a Representative Volume Element (RVE) consisting of 27 grains is introduced. Five grain orientation sets are introduced, where each grain is modelled by a single finite element. To simulate Nanoflex™ texture, 18 Goss and 9 copper grains have been introduced, as these orientations have been observed with OIM in this material with a ratio of 2:1 [8]. The response of a polycrystal resembles clearly a mix of the individual responses of Goss and copper orientations. The drop in reaction stress is alleviated due to the presence of copper orientations, which show a less significant drop. In order to study the interaction of the orientations, the positions of the grains within the RVE have been changed three times. The positions of the grains in the RVE seem to have no effect on the polycrystalline result, i.e. it does not matter where the grains in the RVE are located or if more grains of the same orientation are positioned next to each other. Although the Goss and copper orientations have been subjected to a 5 degree random rotation around their specific Euler angles, the same variants are triggered as in the single grain simulations.

Two other orientation sets of 27 grains are introduced: a mix of Goss and copper grains complemented with some randomly oriented grains and a completely random RVE. All sets of grains show the same qualitative response, however the drop in stress at the onset of transformation becomes less if more randomly oriented grains are present. The reason is that more transformation systems are activated and thus produce martensitic plates (and deformation) in more directions thereby alleviating the drop in reaction stress.

Uniaxial compression analysis of a polycrystal also shows a drop in reaction stress due to transformation. This indicates that the TRIP-effect in compression can also be modeled with the current material model. It has been shown in experiments [12] that compression leads to less transformation than in tension, which is in correspondence with the model predictions. Different transformation systems are active in compression, compared to tension proving that the variant selection principle in the model works properly.

6.1.3 General conclusions

From polycrystalline simulations it can be concluded that the martensite growth predicted by the model is in correspondence with experimental results: the S-shape like martensite evolution during a tensile test is predicted reasonably well. However, the stress-strain curve of a
polycrystalline RVE deviates significantly from experimental curves, with the most remarkable point being the extreme drop in reaction stress at the onset of transformation. Apart from this, the model behavior is in qualitative agreement with experimental material behavior: at the start of transformation the dilatation and shear strain accommodate the externally prescribed displacement and thereby relaxing the stress. Upon increasing martensite volume fraction the composite effect is observed, i.e. the more martensite is present the more the material behavior is dominated by the stronger martensite phase.

The same quantitative deviation from experiments is observed in compression, a drop in stress is also present though smaller. Qualitatively, the results are promising as it has been proven that uniaxial compression also initiates transformation but to a smaller degree.

The core-phenomena behind material behavior in the current material model is variant selection. The activation of specific variants is not explicitly defined but follows from evaluating the energies in the lamella due to deformation and transformation of the phases. By studying the variant behavior under different loading conditions it can be concluded that variant selection works properly: tension of a Goss oriented grain result in significantly different variant behavior than compression. It has been shown that the externally applied stress plays a role in variant selection, but interaction with plasticity is the common denominator, as not always the transformation system is activated in accordance with the simplified theory of Patel and Cohen [12]. This proves that the incorporation of the interaction between transformation and plasticity largely determines model predictions.

6.2 Recommendations

In polycrystalline simulations no interaction between grains has been observed. A constant stress and strain state in the linear finite elements used in discretization possibly forces elements to respond regardless of its surrounding grains and varying stress fields. It is recommended to verify current simulations with higher-order elements and/or (many) more linear elements to describe one grain orientation in a polycrystal. This allows a grain to adjust the response in relation with adjacent grains and varying stress fields. It has been shown in this report that 27 randomly oriented grains is computationally the same as 216 random grains. When higher-order elements are used a similar test should be performed.

Variant selection in the current model occurs without explicitly defining it, but when thermodynamic driving force exceeds a critical barrier. The variants in the current model are activated by basically two mechanisms: (i) externally applied stress and deformation, and (ii) interaction between transformation and plasticity. The verification of variant selection to be found experimentally in the Nanoflex™ material and comparison with the material model should be a recommendation as a result from this work. This is an essential part for evaluating the material model as variant selection largely defines the model predictions.

In the present model the crystallographic orientations of possible transformation variants have been assumed according to the WLR crystallographic orientations of martensite transformation [17]. The applicability of the WLR theory to the Nanoflex™ material, however, still remains to be verified. After the possible transformation variants have been properly identified, the variant activation due to external stresses and local plasticity should also be verified experimentally. Note, however, such experiments are not straightforward and will involve elaborate OIM analysis.

It should be noted that material models of austenite and martensite have influence on
the local plastic flow of the phases, and thus can influence the variant selection in the model as well. If the specific variant selection has been experimentally identified for Nanoflex™ different material models can be tested. Due to the interaction with the transformation, significantly different variant selection is possible for example with crystal plasticity.

Although the material phenomena are modeled qualitatively correctly, quantitative deviation still exists between model results and experiments. This is especially the case for the stress response of a polycrystal. To obtain realistic model predictions, model input should contain more statistical variance of model parameters deviating inter-granular. Statistical deviation can for instance be applied to the transformation barrier function and the elastoplastic model input parameters. A variation in the transformation barrier function of grains would cause the drop in stress, mentioned in this report, to be alleviated and thus result in more realistic model predictions. Furthermore, the transformation barrier function is phenomenologically based on experimental observations. The function is in this report related to the stress-strain behavior of a polycrystal, i.e. the choice of transformation barrier function largely dominates stress-strain behavior. Whether the choice of the barrier function is sufficiently correct remains to be verified. Adjusting the transformation barrier function could quantitatively improve the model predictions.

In current implementation the deformation of the variants is equal, as a result of the Taylor assumption used. Therefore interaction between variants is not included. Other polycrystal homogenization methods for the description of variant deformation can be adopted to ensure variant interaction.

Several computational difficulties were encountered when higher-order elements were used and when the amount of degrees of freedom increased within the RVE. One reason could be a lack of numerical consistency of the model stiffness tensor. The correctness of the material tangent stiffness matrix should be additionally tested by numerical differentiation.

The attractive characteristic of the present material model is that material descriptions of the phases can be easily modified. It is well-known that phase transformation is temperature and strain rate dependent [13] and extension to thermal- and time dependent models would be an improvement. Further, implementing different material models of the phases could result in completely different overall behavior due to different variant selection. For instance, crystal plasticity could initiate completely different variant behavior due to the interaction of transformation and directional plasticity. When the plastic deformation complies with the slip systems of the crystal, different transformation behavior is expected. Also, deformation of materials described with crystal plasticity results in a lattice reorientations and thus change the orientation of a variant, which could then become more preferable for transformation.
Bibliography


Appendix A

Notation

A Cartesian coordinate system applies on the following given vectors and tensors. A unit base \{\vec{e}_1, \vec{e}_2, \vec{e}_3\}, and summation over the indices \(i = 1, 2, 3\) holds.

Quantities

\begin{itemize}
    \item \(a\) scalar
    \item \(\vec{a}\) vector
    \item \(\mathbf{A} = A_{ij}\) second-order tensor
    \item \(^{4}\mathbf{A}\) fourth-order tensor
\end{itemize}

Operators

\begin{itemize}
    \item \(\vec{a} \otimes \vec{b} = a_i b_j \vec{e}_i \vec{e}_j\) dyadic product
    \item \(\mathbf{A} \cdot \mathbf{B} = A_{ij} B_{jk} \vec{e}_i \vec{e}_k\) inner product
    \item \(\mathbf{A} : \mathbf{B} = A_{ij} B_{ji}\) double inner product
    \item \(\mathbf{A}^T = A_{ij}^T = A_{ji}\) transpose
    \item \([a] = a_A - a_M\) jump
    \item \(\langle a \rangle = \frac{1}{2}(a_A + a_M)\) average
\end{itemize}

Subscripts

\begin{itemize}
    \item \(i = A, M\) phases austenite, martensite
    \item \(e\) elastic
    \item \(p\) plastic
    \item \(G\) grain level
    \item \(k\) transformation system level
    \item \(c\) crystal spatial level
    \item \(l\) lamella spatial level
\end{itemize}
Symbols

\( T_0 \)  
\( T_0 \) austenite/martensite equilibrium temperature [K]

\( M_s \)  
\( M_s \) martensite start temperature [K]

\( U_s \)  
\( U_s \) mechanical driving force at \( M_s \) [J]

\( G \)  
\( G \) chemical driving force for transformation, [GPa]

\( G_c \)  
\( G_c \) critical chemical driving force, [GPa]

\( G_c^0 \)  
\( G_c^0 \) initial critical chemical driving force, [GPa]

\( U \)  
\( U \) work by transformation [J]

\( \delta \)  
\( \delta \) dilatation component of transformation

\( \gamma \)  
\( \gamma \) shear component of transformation

\( \vec{F}^{tr} \)  
\( \vec{F}^{tr} \) transformation deformation gradient tensor

\( \bar{N} \)  
\( \bar{N} \) normal of habit plane

\( \bar{M} \)  
\( \bar{M} \) shape deformation vector

\( \varepsilon \)  
\( \varepsilon \) true strain, [-]

\( \sigma \)  
\( \sigma \) Stress, [Pa]

\( \mathbf{F} \)  
\( \mathbf{F} \) deformation gradient tensor

\( \mathbf{P} \)  
\( \mathbf{P} \) first Piola-Kirchhoff stress, [GPa]

\( \xi \)  
\( \xi \) martensite volume fraction, [-]

\( V \)  
\( V \) volume

\( \mathbf{I} \)  
\( \mathbf{I} \) second-order unit tensor

\( 4\mathbf{I} \)  
\( 4\mathbf{I} \) fourth-order unit tensor

\( 4\mathbf{I}^s \)  
\( 4\mathbf{I}^s \) fourth order symmetric unit tensor

\( \mathbf{F}^e \)  
\( \mathbf{F}^e \) elastic part of the deformation tensor

\( \mathbf{F}^p \)  
\( \mathbf{F}^p \) plastic part of the deformation tensor

\( \varepsilon_p \)  
\( \varepsilon_p \) plastic strain, [-]

\( \tilde{\varepsilon}_p \)  
\( \tilde{\varepsilon}_p \) plastic strain prior to transformation, [-]

\( \tilde{\mathbf{F}}^p \)  
\( \tilde{\mathbf{F}}^p \) plastic deformation prior to transformation, [-]

\( [[\psi]] \)  
\( [[\psi]] \) difference of free energies between austenite and martensite, [GPa]

\( \mathbf{B} \)  
\( \mathbf{B} \) left Cauchy-Green (Finger) tensor

\( \tau \)  
\( \tau \) Kirchoff stress tensor, [GPa]

\( 4\mathbf{H} \)  
\( 4\mathbf{H} \) Hookean isotropic elasticity tensor

\( \lambda \)  
\( \lambda \) Lamé’s first parameter

\( \mu \)  
\( \mu \) Lamé’s second parameter

\( \tau_{eq} \)  
\( \tau_{eq} \) equivalent Von Mises stress, [GPa]

\( \tau_y \)  
\( \tau_y \) yield stress, [GPa]

\( \tau_{dy} \)  
\( \tau_{dy} \) deviatoric Kirchoff stress, [GPa]

\( \tau_y^0 \)  
\( \tau_y^0 \) initial yield stress, [GPa]

\( \tau_y^\infty \)  
\( \tau_y^\infty \) infinite yield stress, [GPa]

\( h \)  
\( h \) hardening parameter, [GPa]

\( \eta \)  
\( \eta \) volume fraction of a domain, [-]

\( c \)  
\( c \) proportionality coefficient regarding domains
<table>
<thead>
<tr>
<th>Abbreviations</th>
<th>Full Form</th>
</tr>
</thead>
<tbody>
<tr>
<td>TRIP</td>
<td>TRansformation Induced Plasticity</td>
</tr>
<tr>
<td>FEA</td>
<td>Finite Element Analysis</td>
</tr>
<tr>
<td>RVE</td>
<td>Representative Volume Element</td>
</tr>
<tr>
<td>OIM</td>
<td>Orientation Imaging Microscopy</td>
</tr>
<tr>
<td>FCC</td>
<td>Face Centered Cubic</td>
</tr>
<tr>
<td>BCT</td>
<td>Body Centered Tetragonal</td>
</tr>
<tr>
<td>Philips DAP</td>
<td>Philips Domestic Appliances and Personal Care</td>
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Appendix B

Single grain: multiple elements

In the following Goss and copper orientations are described by 27 elements in an RVE and loaded in uniaxial tension. Two cases are considered: 27 8-node brick elements and 27 20-node quadratic elements, resulting in four calculations. In figure B.1 the RVE is shown.

\[
\mathbf{F} = 1.3 \vec{e}_1 \vec{e}_1 - 0.012 \vec{e}_1 \vec{e}_2 - 0.017 \vec{e}_1 \vec{e}_3 + 0.889 \vec{e}_2 \vec{e}_2 + 0.008 \vec{e}_3 \vec{e}_2 + 0.878 \vec{e}_3 \vec{e}_3 \quad (B.1)
\]

This is caused by the un-symmetric positioned variants with respect to the loading axis. In chapter 4 this is depicted in figure 4.4.
Figure B.2: True stress-strain (a) and martensite fraction-strain curves(b) for Goss and copper: single element responses and RVE’s containing 27 linear and 27 quadratic elements.
Appendix C

Polycrystalline simulations: comparative analysis

A calculation is executed to verify whether 27 grain orientations, used in previous calculations, is representative of the polycrystalline material model response. An RVE consisting of 216 randomly oriented grains (see orientations in Fig. C.1), each grain modelled with one linear finite element is loaded in uniaxial tension. In chapter 5 the result of 27 random orientations was presented, and is here compared to the result of the RVE containing 216 random grains.

Figure C.1: 001 pole figure of 216 random orientations
Figure C.2: (a) True stress-strain curves of 27 random grains vs. 216 random grains, (b) corresponding martensite growth.

From figure C.2 it can be concluded that polycrystalline material model behavior can be correctly modeled with only 27 elements, which verifies analysis in previous chapters. An increase in the number of randomly oriented grains does have very little effect on the macroscopic result.
Appendix D

Pole figures

Pole figures are used to describe the crystallographic texture in materials. A pole figure is a graphical representation of the orientation of objects in space. Pole figures are drawn in the sample reference frame, the orientation relationship between the object and sample can be read from the poles depicted.

A pole figure is set up by considering an object (grain), as in the right part of figure D.1. In this case, a unit cell is transferred to the center of a unit sphere, maintaining it’s relative position to the sample coordinate axis. The pole figure requires that normals of each face of the cube are drawn until intersection occurs with the upper hemisphere. Then, lines connect these intersections with the “south pole” displayed in the left part of figure D.2. When these lines subsequently break through the equatorial plane, poles are drawn. A 2D-representation (right of fig. D.2) then uniquely defines the orientation of one object in 3D-space. Two dominant orientations occurring in this work are Goss and copper. Miller indices of these

Figure D.1: Left: Grain transferred from sample axis to unit sphere. Right: Sample axis with grain orientation. Courtesy of http://aluminium.matter.org.uk
orientation are

\[
\begin{align*}
\text{Goss} & = (1\ 1\ 0) \ <\ 0\ 0\ 1 > \\
\text{copper} & = (1\ 1\ 2) \ <\ 1\ 1\ 1 >
\end{align*}
\]

which can be converted into pole figures (fig. D.3).

Figure D.3: Pole figures of Goss orientation (a) and copper orientation (b)
Appendix E

Representative Volume Element and homogenization

Materials are heterogeneous on the micro-level, where different phases and impurities exist. To characterize the macroscopic material response with sufficient accuracy, these phases have to be taken into account. To predict the mechanical properties of heterogeneous materials ongoing use is made of RVE’s (Representative Volume Elements) combined with homogenization averaging theorems. This allows efficient computational modeling while at the same time representing the deforming microstructure realistically. The repetitive volume element can be defined as the smallest repetitive portion of the material microstructure whose properties are representative of the macroscopic behavior. A prerequisite for RVE modeling is that the constitutive behaviors of the existing phases have to be known. The RVE is then loaded what leads to a response of the different phases on the micro-level. Via homogenization techniques the micro-mechanical response is calculated and will contribute to the engineering (macro) level response. The obtained homogenized constitutive behavior acts as material point (integration point) behavior in finite element techniques.

On RVE-level the problem is reduced to a standard quasi-static continuum equation. The RVE is in equilibrium which is reflected by the static equilibrium equation in the absence of body forces:

\[ \nabla \cdot \mathbf{P}_m = 0 \]  \hspace{1cm} (E.1)

with \( \mathbf{P}_m \) the stress and \( \nabla \) the gradient operator in the micro-structural phases.

The macroscopic deformation of an RVE is given by \( \mathbf{F}_M \). One can load an RVE on different ways, for instance imposed displacements, tractions or periodic boundary conditions. Given an RVE, periodic boundary conditions prove to give the best estimation of the macroscopic properties.

Periodic boundary conditions for a 3D RVE means that opposite surfaces (nodes) should equal their deformation added with the deformation subjected. Or differently said, 4 nodes are prescribed and remaining nodes on opposing surfaces are linked and move simultaneously. Deformation applied to 4 corner nodes (1,2,4,5), with the position vectors \( \vec{x} \) and \( \vec{X} \) in the deformed and undeformed configuration, result in:

\[ \vec{x}_p = \mathbf{F}_M \cdot \vec{X}_p, \quad p = 1, 2, 4, 5 \]  \hspace{1cm} (E.2)
where the nodes can be seen in figure E.1. In this case a schematized uniaxial tensile test is illustrated, motivated by the polycrystalline simulations in chapter 5 which are loaded in this manner.

![Figure E.1: 3D periodic boundary conditions, tensile test.](image)

The $\Gamma_i, \ldots, i = R, L, B, T, F, Back$ stand for the surface of the RVE on the Right, Left, Bottom, Top, Front and Back respectively. Periodically connecting the opposite nodes, while applying deformation on the corner nodes results in the following equations:

$$\mathbf{X}^T - \mathbf{X}^B = \mathbf{F}_M \cdot (\mathbf{X}^5 - \mathbf{X}^1) \quad (E.3)$$

$$\mathbf{X}^R - \mathbf{X}^L = \mathbf{F}_M \cdot (\mathbf{X}^2 - \mathbf{X}^1)$$

$$\mathbf{X}^F - \mathbf{X}^{Back} = \mathbf{F}_M \cdot (\mathbf{X}^4 - \mathbf{X}^1)$$

The resulting macroscopic stress is obtained by adding the external reaction forces $\mathbf{f}$ at the prescribed corner nodes

$$\mathbf{P}_M = \frac{1}{V_0} \sum_{p=1,2,4,5} f_p \mathbf{X}_p \quad (E.4)$$

Finally it should be said that the tangent does not have to be attained by differentiating stress-strain relationship at every point, rather, it follows from condensation of microstructure stiffnesses.