Crystal plasticity based predictions of mechanical properties from heterogeneous steel microstructures

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Abstract. An accurate understanding of the influence of the microstructure on mechanical properties as well as how the material behaves in forming tests is vital for product development and process improvement. The heterogeneity of the microstructure is very different for the various families of steel grades. As a consequence spatial stress and strain distributions on the micro scale will also differ a lot in these materials during forming operations. In the important family of Dual Phase (DP) steel grades, the combination of ductile ferrite phase and hard martensite particles enables an excellent hardening behaviour. However these micro constituents also result in a strong locally heterogeneous behaviour caused by the high material property contrast. To enable an accurate prediction of the materials response in forming processes advanced microstructure models as well as fast crystal plasticity code is essential. Within Tata Steel both are available. A Multi-Level Voronoi microstructure generator, capable of generating very complex Representative Volume Elements, is directly connected to the DAMASK code of the Max Planck Institut für Eisenforschung. This crystal plasticity software is based on an ultrafast Fourier Spectral Solver. Crystal plasticity simulations with different loading cases (e.g. uni-axial, plane strain, simple shear) study various effects of microstructure heterogeneity on stress and strain distributions as well as on global hardening behaviour. Outcome is that not only the volume fraction but also the spatial distribution of the martensite particles has a large impact on local stresses and strains as well as on average hardening behaviour. Another important heterogeneity parameter is the carbon content, which influences strongly the hardness and hardenability of the martensite particles. An attempt is made to incorporate also this effect in crystal plasticity simulations.

1. Introduction

Many different automotive body parts are used in the automotive industry. Because of the differences in shape and functionality a wide variety of, often conflicting, requirements on strength, forming behavior, crash performance and fatigue have to be met. New requirements in the automotive industry demand also for faster product development. In this area Dual Phase steels, consisting out of a soft and a hard phase, are a very important family of steel grades. The soft ferrite phase is responsible for the ductility while the hard martensite particles give these steels their strength. In order to reduce testing computational tools are vital for fast product development. For accurate prediction of mechanical properties still several challenges has to overcome. Firstly one should have a versatile software tool to generate fast many different realistic microstructures. Secondly one should have a crystal plasticity code which is accurate and capable of performing simulations within reasonable amount of time. A typical Dual Phase microstructure consist out of very complex shaped grains surrounded by martensite particles.
Important other characteristics of the microstructure are the volume fraction of the phases, the size distributions of grains and particles, their spatial distributions as well as the micro texture of the grains. For this reason Tata Steel has developed new software which can generate complex Representative Volume Elements (RVE’s), considering above mentioned characteristics, within minutes. These RVE’s are directly connected to a very fast crystal plasticity code, which is based on Fourier transformation. The power of the combination of both multiscale tools will be briefly shown in this paper with several examples. First some details about the microstructure generator will be explained. Then is discussed a new practical method how to assign correct values to crystal plasticity parameters of the individual phases if the chemical composition changes. The mechanical properties of the phases depend strongly on the chemical composition. In the last example we show that the besides the chemical composition also the spatial distribution of the hard martensite particles has a large impact on the hardening behavior of Dual Phase steels.

2. The Multi-Level Voronoi microstructure generator
To be able to construct an extensive range of different microstructures for modern steel grades Tata Steel developed software which algorithm is based on a Voronoi tessellation [1], but has been extended with a lot of features to be able to study many different microstructure configurations. More details of this can be found in [2] and [3].

2.1. Important features
With the multi-level algorithm it is possible to create complex shaped grains in contrast with standard Voronoi, which is only capable of creating convex shaped cells. Different size and spatial distributions for ferrite grains and hard phases can be generated. In the figure 1 below we show 3 RVE’s with a periodic geometry for a Dual Phase steel grade with 19.8%, 39.9% and 60% volume fraction of martensite. The ferrite grains has been assigned Euler angle orientation represented in the figure by different shades of grey. This RVE has been built with 72000 Voronoi cells which has been used to generate 302 complex shaped grains in a cube of 50\(\mu\)m\(^3\). Despite its complexity it takes less than 30 minutes to construct the complete RVE.

![Figure 1: Artificial Dual Phase microstructures constructed with the multi-level Voronoi microstructure generator with 19.8%, 39.9% respectively 60% volume fraction of martensite.](image)

The orientations of the grains have been assigned using EBSD data from industrial Dual Phase material. Using standard smoothing and averaging algorithms available in the EBSD software the original pixels are grouped into grains. Every grain has been assigned one unique orientation. Size and orientation data can then be used to assign orientations to the grains in the 3D RVE. According to Bunge [4] a texture can be described with an orientation distribution function \(f(g)\), which is defined with
\[
\frac{dV}{V} = f(g)dg 
\]

In this \(dV\) are the volume elements with orientation \(g\) in orientation element \(dg\). \(V\) is the sample volume and \(\varphi_1, \phi, \varphi_2\) are the Euler angles. We determine the orientation distribution function from the following simple stereological equation:

\[
\frac{dV}{V} = \frac{dO}{O} 
\]

In this \(dO\) is the area of a grain and \(O\) is the total scanned area of the EBSD scan. Finally a Monte Carlo optimization procedure is used to map orientations to grains in that way that the volume fraction of each orientation comes as closely as possible to the area fraction of the same orientation in the EBSD scan.

2.2. Connection to FFT (Fast Fourier Transform) crystal plasticity solver of DAMASK

In order to be able to perform crystal plasticity simulations on complex microstructures our microstructure generator is directly linked to a FFT crystal plasticity solver in DAMASK. This is open source software developed by the Max Planck Institut für Eisenforschung in Düsseldorf. In [5] it is shown that this software is extremely fast compared to conventional Finite Element methods. This enables us to study the influence of a broad range of microstructures on the mechanical properties. In [6] and [7] an extensive overview has been given about the possibilities.

For our simulations we used the phenomenological material model based on Schmids Law, which describes that plastic deformation will occur on a slip system when the resolved shear stress exceeds a critical value. According to this model shear will evolve on slip systems at a rate

\[
\dot{\gamma} = \dot{\gamma}_0 \left| \frac{\tau_c}{\tau_s} \right| \text{sgn}(\tau_c) 
\]

where \(\dot{\gamma}_0, \tau, \tau_c\) are the reference shear rate, saturation stress and the critical resolved shear stress respectively. The shear stresses evolve asymptotically towards the saturation stress \(\tau_s\).

\[
\tau_c = q_{\alpha\beta} h_0 \left(1 - \frac{\tau_c}{\tau_s}\right)^a |\dot{\gamma}| 
\]

where \(q_{\alpha\beta}, h_0, a\) are slip hardening parameters.

This crystal plasticity model we used for the ferrite phase as well the martensite phase.

3. A practical solution for the determination of crystal plasticity parameters for individual phases

The values of the parameters used in the phenomenological crystal plasticity model are mostly based on fitting procedures for forming simulations on dedicated nano-indentation experiments. For industrial R&D these experimental facilities are often not available. Moreover the constituents of different steel grades will likely have a different chemical composition. It would therefore be much too time consuming and costly gathering crystal plasticity data from these experiments each time we want to perform simulations for another steel grade. Instead we use an approach with uni-axial tensile simulations to determine the crystal plasticity parameters \(h_0, \tau, \tau_c\) from a procedure minimizing the sum of the squares of a set of equations:

\[
\min \left\{ \sum \left[ \sigma(h_0, \tau_0, \tau_s, \varepsilon_{SP}) - \sigma_{SP} \right]^2 \right\} 
\]

where \(\varepsilon_{SP}\) and \(\sigma_{SP}\) vectors containing the individual strain and stress values of an experimental flow curve.
Goal for us is to derive analytical relationships between these crystal plasticity parameters and the chemical composition of the steel grade. In the case of Dual Phase steel, which consists out of ductile ferrite grains and hard martensite particles, the mechanical properties of martensite are strongly influenced by the carbon content. Martensite consisting out of more carbon will be harder. In order to incorporate this effect in our crystal plasticity model we used an analogue approach as described by Rodriguez in [9]. In this paper has been described how hardening curves of ferrite and martensite can be related to their chemical composition. Moreover with data from the experiments described in [10] we are able to derive directly a relation between volume fraction of martensite, its carbon content and the crystal plasticity parameters \( \tau_s \), \( \tau_c \), \( h_0 \). In figure 2 it can be seen that the relations for all 3 parameters are almost perfect linear. Using this procedure we are now able to perform more accurate simulations in a broad range of dual phase steels with many different volume fractions of martensite.

In figure 3 it can be seen, as expected, that higher volume fractions of martensite will give a harder response in uni-axial tensile tests. The average carbon content in martensite is lower in microstructures.
with higher volume fractions. This effect could be successfully incorporated within our relations for crystal plasticity $h_0$, $\tau_s$, $\tau_c$. Results show a lower response for dual phase material with higher volume fractions of martensite and a higher response in case of dual phase material with lower fractions of martensite.

4. Parametric study: The influence of the spatial distribution of the martensite particles in Dual Phase steel grades

A big advantage of a microstructure model is that we are able to study very fast different aspects of microstructures, which are very hard to produce in experimental materials. In the study in figure 4 the microstructures are produced within hours and the crystal plasticity simulations took together a few days.

![Random and Network Microstructures](image)

In this case we want to study the influence of the spatial distribution of martensite. We created to different dual phase microstructures with 20% and 39% volume fraction of martensite. In both cases with a random distribution as well as martensite situated only along ferrite grain boundaries (network). For reasons of comparison we kept every other property has the same. We took the size ratio ferrite grains versus martensite particles higher than what one would normally observe in industrial dual phase microstructures. This has been done to study a closed network effect already occurring at relative low volume fractions of martensite. In figure 5 one can see the hardening responses of the RVE’s after maximal 20% deformation by an uni-axial tensile test. Higher fractions of martensite will result, as expected, in higher hardening responses. Another conclusion is that if martensite particles are spatially connected in a network this will give an extra hardening effect on the total response. This effect, which is getting more attention, is stronger for higher volume fractions of martensite. For our simulations we took a random orientation distribution of martensite. One of our next steps will be to assign specific
orientation distributions to the martensite particles in a closed network configuration and study the influence of this combination on the stress and strain response after uni-axial tension deformation.

Figure 5: Comparison of hardening response (in MPa) between Dual Phase microstructures with randomly distributed martensite and martensite in a network at ferrite grain boundaries.

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