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Microstructure Effects on the Plastic Anisotropy of a Fine-Structured Dual-Phase Steel

Wenqi Liu and Junhe Lian

Abstract

In sheet metal applications, the plastic anisotropic behavior of metallic materials is significantly important, which is affected by the nature of deformation mechanisms with orientation dependency and the microstructure morphology. This study performs a numerical investigation on the anisotropic behavior during plastic deformation affected by the microstructural features. An automotive high-strength fine-structured dual-phase steel (DP1000) is selected as the reference material. The focused microstructural features are phase fraction, grain shape, and crystallographic orientation. The coupling of the fine-resolution representative volume element (RVE) method and the crystal plasticity (CP) model is employed to consider the material microstructural features and to predict the plastic response at the macroscopic level. An optimal RVE is built for the reference material. The modeling approach is validated by the anisotropic predictions of uniaxial tensile tests along material rolling, diagonal, and transversal directions (RD, DD, TD). Then a set of RVES with varying phase fraction, grain shape, and crystallographic orientation is generated and works as a virtual laboratory to investigate the influence of microstructural features on anisotropic behavior of dual-phase steel.

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Keywords: Dual-phase steel; Anisotropy; Crystal plasticity finite element method; Representative volume elements

1. Introduction

The advanced high strength steels (AHSS), for example, the dual-phase (DP) steels, are widely used in industry, especially in the automotive industry for lightweight design. This is benefited from their mechanical advantages, such as the attractive combination of strength and formability. It is well known that the mechanical properties of steels are determined by the microstructure. Therefore, for material design, the understanding of the quantitative relationship between the material microstructure and its properties, in particular, the plastic anisotropic behavior, is of high interest for the sheet metal production and forming industry. Recently, the integrated computational materials engineering (ICME) approach is widely used as a reliable and efficient strategy for linking the microstructure and mechanical property and further developing the material that fulfills the desired component mechanical performance.

There has been a large number of studies focusing on bridging the microstructure and macroscopic mechanical properties by both experimental and numerical methods. The interested microstructural features normally are the phase fraction, grain morphology, crystal orientation, secondary phase morphology, etc. While the focused mechanical properties can be various from microscopic level strain partition, macroscopic flow behavior, to fracture and fatigue properties, etc. For example, Li [1] discussed the microstructure induced strain partitioning and heterogeneity in full bainitic, complex-phase and dual-phase steels. Lopes, Barlat, et al. [2] studied the texture and dislocation structure linking the microstructure and mechanical property and further developing the material that fulfills the desired component mechanical performance.
effects on the anisotropy of strain hardening of an aluminum alloy. Pierman, Bouaziz, et al. [3] investigated the flow properties of DP steels, including yielding, tensile strength, and ductility, by varying the martensite volume fraction, carbon content and morphology. Li, Golden, et al. [4] developed a multiscale modeling framework to observe the effects of the precipitate size on overall stress-strain response and plastic strain localization in martensitic steel. Han, da Silva, et al. [5] used experiments to study the effects of prior austenite grain boundaries and microstructural morphology on the impact toughness of medium Mn steel. Diehl, Groeber, et al. [6] employed the microstructure and material modeling to build the microstructure-property relationship of high Mn steel. Among these investigations, it is well noted that in the numerical simulation based on the crystal plasticity (CP) models in the form of either full-field finite element method [7-11], or the mean-field visco-plastic self-consistent (VPSC) models [12-15] are well developed to bridging the crystal microstructure and its mechanical properties.

Although various experimental and numerical studies have been conducted to study the material microstructural and mechanical anisotropy, a systematic and qualitative investigation on the effects of individual or integrated microstructural features on the plasticity anisotropy in terms of strength and R-value has not been well reported. This measure could be of significant importance for the material and structure design point of view. It is quite a challenge to produce these data using the experimental method, as the microstructure features are hard to be varied based on a single-variable concept. Therefore, using the ICME concept could deliver such a comprehensive database with better control over the influencing variables. However, for the fine-structured high-strength DP or complex-phase steel, the challenges that hinder such an investigation arise from the following two aspects: i) the fine-resolution synthetic microstructure modeling to accurately represent the material microstructure and precisely control the microstructural variables, and ii) the efficient and reliable material parameter calibration for each individual phases in the DP or multi phases steels. To solve these two challenges, Liu, Lian, et al. [16] have developed a strategy for generating the synthetic microstructure and calibrating the crystal plasticity parameter of fine-grain-structured DP steel, which could enable a systematic and quantitative analysis of the influence of microstructure features. Based on this study, the synthetic microstructure models, i.e. representative volume element (RVE) models, can be generated with desired microstructural feature requirements including phase fraction, grain shape, and crystallographic orientation. Coupling with crystal plasticity model and calibrated material parameters, a virtual laboratory is built up and virtually uniaxial tensile tests under material rolling, diagonal, and transversal directions (RD, DD, TD) are carried out to quantitatively assess the influence of the microstructural features on anisotropic behavior of DP steel.

2. Material

A DP1000 is employed in this study as the reference material. To prudently and comprehensively analyze the microstructure, the light optical microscopy (LOM), scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD) techniques are used. The investigated DP1000 is comprised of 55% ferrite and 45% martensite with very fine grains. The average grain size of ferrite is around 2.0 μm and martensite is ~0.5 μm. The grain orientation distribution for both phases has the typical rolled texture components. For ferrite, the γ-fiber is the dominant texture fiber, while for martensite the rotated-cube component is the most important one. The detail microstructure characterization program and results of the DP steel are referred to Liu, Lian et al. Liu, Lian, et al. [16].

3. Modeling

3.1. Crystal plasticity

The crystal plasticity model with the phenomenological constitutive laws is used in this study. It is noted that with the phenomenological crystal plasticity model, the size effect can be not rendered. However, the morphology effect, including both phase and crystal levels, can be taken into account with the full-field computational homogenization methods. The DAMASK (Düsseldorf Advanced Materials Simulation Kit) platform with the multiscale material point model [7] is used in the study. The solved boundary condition is in the form of an average deformation gradient and the material point model is employed to provide the corresponding average first Piola-Kirchhoff stress. In an RVE case, the material point is a polycrystalline aggregate and the average deformation gradient has to be partitioned into individual deformation gradients for each crystal in the RVE. As a return quantity, the individual crystal stress has to be homogenized into the average stress of the RVE. Then, on the crystallite level, the constitutive laws are employed to solve the elastoplasticity problem in terms of the plastic velocity gradient as a function of the second Piola-Kirchhoff stress. The plastic velocity gradient $L_p$ can be defined as:

$$L_p = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha m^\alpha \otimes n^\alpha$$

(1)

where for slip system $\alpha$, $m^\alpha$ and $n^\alpha$ are the unit vector describing the slip direction and normal direction to the slip plane, $\dot{\gamma}^\alpha$ is the shear rate. N is the number of active slip systems. The shear rate $\dot{\gamma}^\alpha$ is determined by the resolved shear stress $\tau^\alpha$ and the critical resolved shear stress $\tau_c^\alpha$. The kinetic law on the slip system $\alpha$ is given as:

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{\tau^\alpha}{\tau_c^\alpha} \right)^m \text{sgn}(\tau^\alpha)$$

(2)

where $\dot{\gamma}_0$ and $m$ are the reference shear rate and rate sensitivity of slip system $\alpha$ respectively. The resolved shear stress $\tau^\alpha$ on slip system $\alpha$ is defined as:

$$\tau^\alpha = S \cdot (m^\alpha \otimes n^\alpha)$$

(3)

where $S$ is the second Piola-Kirchhoff stress. The micromechanical interaction between different slip systems
shall also be taken into consideration by:

\[ \tau^a_c = \sum_{\beta=1}^{N} h_{a\beta} |y^\beta| \]  

(4)

where \( h_{a\beta} \) is the hardening matrix and given as:

\[ h_{a\beta} = q_{a\beta} \left[ h_0 \left( 1 - \frac{t_\beta^c}{t_\alpha^c} \right) \right]^\alpha \]  

(5)

where \( h_0, \alpha, \) and \( t_\alpha^c \) are slip hardening parameters. The value \( q_{a\beta} \) incorporates the effect of self-hardening (\( \alpha = \beta \)) and latent hardening (\( \alpha \neq \beta \)) and is assigned as 1.0 for coplanar slip and 1.4 otherwise. Therefore, the hardening evolution law of slip system \( \alpha \) is determined according to:

\[ \tau^a_c = \tau_0 + \int_0^t q_{a\beta} \left[ h_0 \left( 1 - \frac{t_\beta^c}{t_\alpha^c} \right) \right]^\alpha |y^\beta| dt \]  

(6)

where \( \tau_0 \) is the initial critical resolved shear stress. In this hardening law, for the quasi-static loading condition without considering the strain rate sensitivity, the involved parameters are \( \tau_0, \tau_\alpha^c, a_0, \) and \( a, \) which need to be calibrated for each phase. It is noted that for each grain and/or phase, on the one hand, the individual response stress is varied based on their crystal orientation and/or the involved crystal plasticity parameters. On another hand, it shall also be homogenized with its neighbors according to the RVE average values. Therefore, excepted for the boundary effect, the phase fraction, grain shape and orientation influence can be considered with phenomenological crystal plasticity models. Besides, it is noted that the chemical composition induced mechanical property change is not considered in the phase fraction influence study.

The fast Fourier transformation (FFT) approach on the DAMASK platform [7] is used in this study to solve the constitutive equations in the crystal plasticity model. It is suitable for the CP simulations with periodic boundary conditions, e.g. the RVE simulations under uniaxial loading, due to its higher numerical performances with the economical computing time and better predictive capabilities as a mesh-free method. The detailed explanations of the scheme and implementation with CP models have been investigated in many studies [17, 18].

### 3.2. Reference RVE generation and parameter calibration

A microstructure representativeness assessment criterion/diagram (MRAC/MRAD) is proposed according to the comparison of the deviations on the individual and global microstructural features between the artificial RVE structure and the experimental measurement in the previous study [16]. This approach can be used to guide the evaluation of the representativeness of the synthetic microstructure and optimize the generated RVEs. Considering the overall microstructural information of the reference material, the mesh size of 0.2 μm with 64,000 (40×40×40) elements are the optimal RVE numerical parameters. This optimal RVE has a size of 8×8×8 μm³, which contains 51 ferrite grains and 1040 martensite grains. In addition, the grain size and orientation distribution of the output RVE are compared and further modified to match the reference material characters as well. The phase map of the optimal RVE is shown in Fig. 1 (45%).

The grain shape factor is defined as the aspect ratio of three specific axes of a grain. Normally, grains are regarded as equivalent ellipsoids in a 3D Cartesian coordinate system, hence, the grain shape aspect ratio is the length ratio of the three ellipsoid coordinate axes, marked as \( a:b:c \). For example, \( a:b:c=1:1:1 \) refers to equiaxed grains. According to the EBSD analyses, the reference DP1000 has a grain shape aspect ratio close to \( 1:0.5:0.5 \) for both phases [16]. In numerical investigation, another four cases are chosen as \( 1:1:1, 1:0.75:0.75, 1:0.25:0.25, \) and \( 1:0.1:0.1 \) for both phases. The exact grain shape factor values are also listed in Table 2 and the...
generated RVEs are shown in Fig. 2. It is noted that in the synthetic microstructural models, the specific coordinate system is unified with the material coordinate system, i.e. RD-TD-ND axes. That means, the grain shape factor can be also characterized as RD:TD:ND.

![Fig. 2. Grain maps of RVEs with different grain shapes [16].](image)

The grain orientation can be represented with several methods, e.g. Orientation matrix, Euler angles, Miller index, Angle-Axis, etc. The rolled body center cubic (bcc) metals tend to form fiber textures [20]. Therefore, the Miller index method can well describe the bcc deformation texture. The most characteristic fibers in bcc metals are α-fiber with <011>//RD and γ-fiber with [111]/ND. Considering their Euler angles range and the cubic crystal symmetry, in Euler space, most important texture features can be seen in the section.

In this study, seven typical texture components are chosen for numerical investigation, as shown in Fig. 3. For each component, orientations differing the misorientation angular tolerance within 15° (referring to the high angle grain boundaries) from this special texture component center are assigned to grains from both phases in the optimal RVE for simulation.

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For strength and strain hardening rate, the differences in the predicted results from variable input settings are close to each other in many cases, especially for the grain shape group. For the better comparison among different microstructure and loading conditions, the normalized parameter $S_{Nor}$ is introduced:

$$S_{Nor} = \frac{Y_{i}}{Y_{Ref}}$$

where $Y$ is the interested mechanical property and $i$ represents the focused microstructural feature. The reference value $Y_{Ref}$ is calculated from the optimal RVE under the RD loading condition, which exhibits the mechanical property of the reference material.

In terms of R-values, the differences among different input settings are much more obvious. Meanwhile, it is noted that the absolute R-values are important for material design. As the R-value close to one is always pursued in most industrial applications. For many cases, R-value larger than one is also preferred, since more deformation in the transverse direction is better than larger strain in the thickness direction. Therefore, the original R-values are employed.

**3.4. Mechanical property characterization**

During plastic deformation, the interested mechanical properties are the flow strength and R-values including their evolution. Coupling the RVE and CP models, both flow curves and R-value evolution curves can be predicted. For the anisotropic study, simulation under the RD-0°, DD-45°, and TD-90° loading conditions are carried out. The examples are shown in Fig. 4. As the uniform elongation of the reference material is close to 5%, the focused characteristics on strength are the yielding stress $\sigma_{0}$ and flow stress at true plastic strain $\dot{\varepsilon}_{p}=0.05$ ($\sigma_{0.05}$). However, for R-values, it is clear that the R-values in the initial plastic deformation stage are not stable. Therefore, R-values at $\dot{\varepsilon}_{p}=0.01$ and 0.05 ($R_{0.01}$ and $R_{0.05}$) are chosen. The distinct R-value evolution can be observed in this range. In addition, the strain hardening rate $\dot{n}$ until $\dot{\varepsilon}_{p}=0.05$ is also focused. All these characteristics are extracted from the predicted flow curves and R-value evolution curves. In the following sections, only these characteristics are presented and employed for discussion.

![Fig. 3. Orientation distribution function figures in the section of investigated typical bcc texture components and the reference material texture.](image)

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**4. Results and discussion**

**4.1. Strength**

As aforementioned, the yield strength $\sigma_{0}$ and flow stress $\sigma_{0.05}$ are used to indicate the strength and its evolution. For each
case, the stress of optimal RVE (with martensite phase fraction of 45% and grain shape factor of 1:0.5:0.5) under RD loading is the reference point. Fig. 5–Fig. 7 reveal the phase fraction, grain shape, and crystal orientation influence on \( \sigma_0 \) and \( \sigma_{0.05} \), respectively.

According to Fig. 5, it is clear that with the increased martensite phase fraction, both the yield strength and flow stress at 5% strain are distinctly enhanced. Furthermore, the increase rate of the \( \sigma_{0.05} \) (close to the reference material UTS) is lower than the yielding strength. This is caused by the different individual mechanical performance of martensite and ferrite, as martensite is the harder phase against stress while ferrite is the softer one, which bears the most strain. Besides, the martensite phase has a smaller global work hardening rate than ferrite. In the phenomenological crystal plasticity modeling, the differences in phase performance are achieved by the different hardening parameters. Furthermore, in the investigated phase fraction range, loading along DD always performs the lowest strength while the TD loading condition shows the highest strength. It is also noted that with the increase of the martensite phase fraction, the anisotropic difference in strength tends to be minimized. In DP steel with complex microstructure and variable texture, the global anisotropic behavior shall be affected by a variety of reasons. Except for the phase-level stress-strain response change, the variable phase fraction also leads to global texture diversification, which might result in comprehensive grain-level interaction. Conclusively, in the strength anisotropy point of view, DP steel with higher martensite phase fraction shall be preferred for material design concerning the yielding and initial hardening.

In terms of grain shape effect in Fig. 6, RVEs with 1:0.1:0.1 shape factor go through the highest strength. However, it is noted that there are many extremely elongated grains running through the whole RVE along RD. Hence, the boundary effect cannot be avoided in this case. Generally, the strength is increased by the decreased grain shape factor in all loading conditions, but only with the slight differences between different groups, especially in the shape factor range from 1:0.5:0.5 to 1:1:1. Compared to the equiaxial sphere, with the decreased grain shape factor, the superficial area of elongated grain is increased, which results in increased grain boundary area and the limited dislocation movement free path. The interaction between different grains is also enhanced and leads to slightly increased RVE global strength. Besides, the strength anisotropic behavior is also weakly affected by grain shape, except for the excessively small shape factors. For both \( \sigma_0 \) and \( \sigma_{0.05} \), RVE 1:0.75:0.75 shows the relatively smaller anisotropic difference around 3%. While for RVE 1:1:1, the anisotropic difference is also smaller than 5%. Therefore, in the grain shape factor range from 1:0.5:0.5 to 1:1:1, the grain shape effects on the strength is not obvious.

The texture effect is exhibited in Fig. 7. It is illustrated that if only single crystal orientation is developed, texture influence on both strength and anisotropy is significantly different. Generally, the texture effects on TD and DD are larger than RD loading. \{112\}<110> performs the highest RD and TD strength, while Goss component \{011\}<100> gives the DD peak strength values on both yielding and tensile strength points. Meanwhile, Goss texture also shows the largest deviation on anisotropic strength while \( \gamma \)-fiber \{111\}<110> and \{111\}<112> performs the weakest anisotropy. Besides, the cube component \{001\}<100> and rotated-cube component \{001\}<110> show minimum strength and the opposite anisotropic tendency with each other. The off-\( \gamma \)-fiber component \{554\}<225> exhibits the same anisotropic behavior with the \( \gamma \)-fiber but with larger anisotropy and generally lower strength except for the DD loading. Furthermore, it can be seen that the stress values of \( \gamma \)-fiber components \{111\}<110> and \{111\}<112> are close to the reference material, while the \( \alpha \)-fiber components \{112\}<110> and \{001\}<110> show the same anisotropic tendency with the reference. According to Fig. 3, these components also are the most important texture in the reference material; therefore, the global strength behavior is related to the combination of these mixture texture components. For applications, the preferred crystal orientation can be picked up for each single/proportional loading case, while for complex loading conditions, the \( \gamma \)-fiber with homogeneous anisotropy and relatively high strength shall be considered.

![Fig. 4. The predicted flow curves (a) and R-value (b) evolution curves of RVEs with different martensite phase fractions under TD loading condition, and (c) the deformed strain pattern of 45% RVE under TD loading condition.](image-url)
4.2. Strain hardening rate

The stress–strain evolution is preliminarily discussed in the last section by comparing the yielding stress \(\sigma_0\) and flow stress \(\sigma_{0.05}\). The strain hardening rate \(n\) is used to assess the global work hardening during the plastic deformation stage. It is defined as the arithmetical mean strain hardening rate from yielding point until \(\varepsilon = 0.05\) [16]. The results are shown in Fig. 8.

Comparing Fig. 5 with Fig. 8, it is demonstrated that the strength and work hardening rate generally have the same anisotropic tendency no matter with which martensite phase fraction, i.e. TD>RD>DD. However, with the increased martensite fraction, the overall work hardening rate is decreased, which is the same as the reduced increase rate on \(\sigma_{0.05}\). As aforementioned, this is caused by the smaller work hardening rate of the martensite phase.

The grain shape effect on work hardening is much more complex as shown in Fig. 9. For RD and DD loading conditions, it is normally increased with the increased shape factor, while for TD, there is no distinctly affected tendency of grain shape factor on work hardening rate. Besides, similar to strength, the grain shape effect in the range from 1:0.5:0.5 to 1:1:1 is very small with the maximum difference less than 6% for each individual loading condition. In this range, RVE with the shape factor of 1:0.75:0.75 has the largest anisotropic difference of 12%, while the equiaxial RVE shows the minimum anisotropic difference of 5%, which shall be better for material design.

In terms of texture effect, comparing Fig. 7 with Fig. 10, it is indicated that most texture components have the same influence on the anisotropic tendency on both strength and work hardening rate, except for \{001\}<100> and \{001\}<110>. They hold the minimum work hardening rate as before but the opposite work hardening anisotropic behavior compared with strength anisotropy. In addition, it is noted that \{112\}<110> still performs the highest work hardening rate under RD and TD loading conditions, while \{011\}<100> gives the DD peak value, that is the same phenomena as the strength. Besides, the Goss component still shows the largest anisotropic difference of up to 40%. Meanwhile, the cube component, rotated-cube component, and \(\gamma\)-fiber components perform the relatively smaller anisotropy, with the difference between three loading conditions less than 10%.
4.3. R-value

The microstructure effect on R-value is indicated by $R_{0.01}$ (close to the initial R-value) and $R_{0.05}$ (close to the uniform elongation), as shown in Fig. 11–Fig. 13. It is worth noting that with the reference texture, no matter how the phase fraction and grain shape change, the anisotropic tendency of R-value almost keeps the same, i.e., the largest R-value occurs under DD loading condition (larger than one) while the smallest one comes from RD (smaller than one). Besides, the R-values under TD loading conditions are generally closer to one. However, in contrary to the tendency of strength, the microstructure induced R-value change is irregular.

Normally, compared to strength, R-value is strongly affected by the crystal orientation and more sensitive to the interaction between grains. The single crystal orientation effect is clearly indicated in Fig. 13. For instance, with texture component changes, the R-value could differ from 0.05 (rotated-cube component) to larger than 20 (Goss component) under TD loading condition. Even under the RD loading condition, which offers a relatively smaller difference, the R-value is changed from 0.05 to a value larger than two with a difference up to 300% (comparing with the reference value). Therefore, in Fig. 11 and Fig. 12, with the RVE structure change in terms of phase fraction and grain shape, it is difficult to keep all RVEs with completely the same texture information as each other. A small difference in RVE texture might cause a distinct deviation on the overall R-value. Especially for phase fraction, as ferrite and martensite hold the different crystal orientation distribution (shown in Fig. 3), the increased martensite phase fraction brings the different combinations of the texture of two phases, which results in the irregular change on R-value and its evolution. What is more, for the deep understanding of the microstructure induced R-value difference, especially for grain shape effect, the single-phase RVE shall be considered to precisely control the microstructure variables and the dislocation-based CP models shall be developed to study the grain boundary effect. In addition, the misorientation distribution shall also be involved to take into account the grain interaction.

Overall, in the phase fraction group, the martensite phase fraction of 60% offers the smallest R-value and R-value anisotropy, which shall be a benefit for material applications. Analogously, in terms of grain shape types, the equiaxial grains carry the same conclusions. In addition, from the texture point of view, the R-values of the γ-fiber components {111}<110> and {111}<112> are larger than one for all three loading conditions, and they perform the minimum R-value anisotropy as well, which is preferred for material design.
The main behavior. Evaluating their mechanical property performances including strength, work hardening rate, and R-value, the phenomenological crystal plasticity model is employed in this study to investigate the effects of microstructure in terms of phase fraction, grain shape, and crystal orientation on the plasticity anisotropic effects of microstructure. For dual-phase steel, higher martensite phase fraction is better for enhancing strength and 60-70% of martensite is optimal. Rolled/elongated grains (1:0.5:0.5) perform higher strength from 1:0.5:0.5 to 1:1:1 is relatively weak. The grain boundary, grain size as well as chemical composition effects. The misorientation influence shall also be considered to involve the grain interaction effects on plasticity anisotropy.

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