Micromechanical Finite Element Analysis of the Effects of Martensite Particle Size and Ferrite Grain Boundaries on the Overall Mechanical Behavior of Dual Phase Steel

This paper focuses on micromechanical finite element (FE) modeling of the effects of size and morphology (particularly elongation or aspect ratio (AR) along the loading direction) of martensite particles and the ferrite grains on the overall mechanical behavior of dual-phase (DP) steels. To capture the size-effect of the martensite particles and ferrite grains, the core and mantle approach is adapted in which a thin interphase of geometrically necessary dislocations (GNDs) is embedded at the martensite–ferrite boundaries. It is shown that as the martensite particles size decreases or their aspect ratio increases, both the strength and ductility of DP steel increase simultaneously. On the other hand, as the ferrite grain size decreases or its aspect ratio increases, the overall strength increases on the expense of the ductility. The conclusions from this study can be used in guiding the microstructural design of DP steels. [DOI: 10.1115/1.4036687]

Keywords: dual-phase steel, microstructural modeling, finite element analysis, martensite morphology, grain boundaries

1 Introduction

Dual-phase (DP) steel is a type of advanced high-strength steels (AHSS), which is commonly used in the automotive industries. They are primary of high strength and good deformability and are relatively very cheap as compared to other types of AHSS. Because of their wide use in manufacturing car parts, the automotive industries are continuously exploring methods of producing newer grades of DP steels with simultaneous increase in the strength and ductility. The overall mechanical behavior is primarily governed by the hard particlelike martensite phase embedded into a softer ferrite phase [1]. More specifically, the volume fraction, morphology (i.e., shape, size, and distribution), carbon content, and grain size also contribute to the overall behavior [2–8].

In the last few years, there have been various attempts in correlating the microstructural parameters to the overall behavior of DP steels through microstructural modeling of representative volume elements (RVEs). In the early works of Al-Abbasi and Nemes [9,10], micromechanical modeling was performed on cells which resembled the martensite phase of DP steels. It was concluded that the effect of size and distribution can be neglected at intermediate and higher V_M, the effect becomes noticeable. In an attempt to predict more realistic results, scanning electron microscopy (SEM) images were used to generate the finite element (FE) models in a series of work by Khalife and coworkers [11–14]. By adapting the classical (local) von Mises plasticity without any damage model, it was concluded that the failure and the softening of DP steels is due to plastic strain localization. Furthermore, several other works have been published that further explore the influence of microstructural parameters on the overall behavior of DP steels (e.g., see Refs. [15] and [16–30]). For extensive review of such micromechanical modeling, studies can be found in Ref. [31].

Despite the intense research efforts, there remain several important key microstructural parameters that have not been investigated in-depth, computationally, in spite of their great influence. This is because the methodology used to mimic DP microstructure, namely: (1) checker-boxes [21,26], (2) circles [10,32], (3) Voronoi cells (e.g., see Refs. [33] and [34]), (4) SEM images [11,14,15], and (5) electron backscatter diffraction (EBSD) images (e.g., see Refs. [28] and [29]), do not allow the user to generate realistic microstructures with all the parameters in the control of the user. Hence, this paper will be focusing on exploring never-done parametric studies on DP steels.

It was shown in the work of Kadkhodapour et al. [35], who used nanoindentation, that the ferrite phase plastically behaves inhomogeneously. This is primarily due to the presence of geometrically necessary dislocations (GNDs) at the interphase of the ferrite and martensite phases. However, most of the aforementioned works have not taken this into account. Moreover, Kadkhodapour et al. [35] and Ramazani et al. [25] attempted to model the interphase between the two phases of DP steels; however, the interphase thickness and mechanical properties were not taken from experimental results. Hence, in this paper, the interphase thickness and its properties are obtained from the microcompression pillar testing that was performed by Ghassemi-Armaki et al. [36].

Another important parameter in micromechanical modeling of DP steels is the grain size of the ferrite phase [37]. It was shown recently in the work of Calcagnotto et al. [38] that the yield and tensile strengths increase without any significant change in the ductility for a smaller grain size in DP steels. This is partially because of the grain refinement process which increases the...
strain-hardening rate through increasing GNDs along the ferrite and martensite boundaries [39]. There are many methods proposed in literature for modeling the grain size-effect. The most commonly used is the well-known Hall–Petch relationship [40], which is based on dislocations pileup at the boundary. This empirical relationship fits a wide range of materials. Despite this relationship, there have been many attempts to model grain size to further enhance the understanding. One of the main continuum-based models used for modeling grain size-effect is the so-called “core and mantle” hardening model (e.g., see Refs. [41] and [42]), in which the grain boundaries are modeled by placing a thin layer or an interphase of finite thickness along the grain boundaries. Another continuum-based approach is the higher-order strain gradient plasticity models through GNDs accumulation at the grain boundaries (e.g., see Refs. [43] and [44]). For simplicity, in this paper, the core and mantle approach is used to incorporate the grain size-effect on the overall response of DP steel. The same approach is also employed to incorporate the martensite phase (particle) size-effect.

Finally, this paper is divided into two main parts. The first part will be focusing on predicting the size-effect of the martensite particles on the overall behavior, while the second part will be focusing on modeling different morphologies of grain boundaries of DP steels. It is important to emphasize here that the previously mentioned studies have not been investigated before thoroughly through computational modeling.

2 Microstructure Modeling

In this section, the microstructural finite element modeling of DP steels is presented. Figure 1(a) represents a virtual RVE generated through a MATLAB code. The MATLAB code is based on the Voronoi tessellation; however, it is implemented with a postalgorithm that generates more realistic microstructures based on the user’s need. The details of this code are presented in Ref. [31]. It is important to emphasize that predicting ductility of DP steel from material inhomogeneity is fully mesh sensitive. However, the authors have performed a comprehensive mesh-sensitivity case study in their previous work [31]. In this study, it was shown that by adopting an elastic–plastic model, the results were mesh sensitive. However, if an elastic–viscoplastic model is implemented the mesh sensitivity issue is resolved, since viscoplasticity introduces an intrinsic length-scale parameter which yields mesh-objective results [45]. Therefore, in this work, the same methodology is used. Further details on this can be found in the authors’ previous work [31]. Moreover, statistical distribution analysis and validation of these microstructures are also presented in the same paper.

Figure 1 represents a virtual RVE that has been converted into an FE model. The analysis software used in this study is the well-known commercial finite element software ABAQUS [46]. In all simulations in this study, plane stress assumption is adapted as DP steels are generally manufactured as thin sheets. The RVEs are meshed with computationally cheaper plane stress quadratic elements with reduced integration (CPS4R) and with hour-glass control parameter of 0.05 in order to avoid shear-locking when using full integration and hour-glass problem when using reduced integration [47]. Periodic boundary conditions are enforced. The applied tensile strain rate is $10^{-3}$ s$^{-1}$ representing quasi-static loading. Each phase in the DP steel is modeled as a finite deformation elastic–viscoplastic material and using von Mises plasticity. Assuming small elastic deformation, the total rate of deformation tensor, $\mathbf{D}$, is additively decomposed as follows:

$$
\mathbf{D} = \mathbf{D}^e + \mathbf{D}^\text{vp}
$$

where $\mathbf{D}$ is the symmetric part of the velocity gradient $\mathbf{L} = \dot{\mathbf{F}} \mathbf{F}^{-1}$, with $\mathbf{F}$ being the deformation gradient and the superimposed dot denotes a material time derivative, $\mathbf{D}^e$ is the elastic component, and $\mathbf{D}^\text{vp}$ is the viscoplastic component. The Jaumann objective rate of the Cauchy stress tensor, $\dot{\mathbf{\sigma}}$, is given by

$$
\dot{\mathbf{\sigma}} = \frac{1}{1+\nu} \left[ \mathbf{D}^e + \frac{\nu}{1-2\nu} \mathbf{D}_{kk}^e \mathbf{I} \right]
$$

where $\dot{\mathbf{\sigma}}$ is the Cauchy stress tensor, $\mathbf{I}$ is the second-order identity tensor.

The viscoplastic flow rule for calculating $\mathbf{D}^\text{vp}$ is given by

$$
\mathbf{D}^\text{vp} = \frac{3}{2} \dot{\varepsilon}_\text{vp} \mathbf{S} \mathbf{\Sigma}
$$

with

$$
\sigma_e = \sqrt{\frac{3}{2} \mathbf{S} : \mathbf{S}}, \quad \mathbf{S} = \sigma - \frac{1}{3} \sigma \mathbf{I}
$$

and

$$
\dot{\varepsilon}_\text{vp} = \Gamma \left( \frac{\sigma}{g} - 1 \right)^{\frac{1}{\gamma}} - \sigma_g + h(\sigma)^n
$$

Here, $n$ is the strain hardening exponent, $m$ is the strain rate hardening exponent, $\sigma_g$ is the yield strength, $\Gamma$ is the inverse of the relaxation time, $h$ is the hardening modulus, and $\langle \rangle$ is the Macaulay bracket. The equivalent viscoplastic strain $\dot{\varepsilon}_\text{vp}$ is defined as

$$
\dot{\varepsilon}_\text{vp} = \int_0^t \sqrt{\frac{3}{2}} \mathbf{D}^\text{vp} : \mathbf{D}^\text{vp} dt
$$

It is important to mention here that a more complicated model such as the crystal plasticity model (e.g., see Refs. [48] and [49]) or the dislocation density-based model (e.g., see Ref. [50]) was not adopted here because of their high computational cost along with their complexity associated in simulating such complex microstructures. Moreover, such models require additional material parameters for calibration for each phase, which is not easily available in literature. Therefore, for simplicity in simulating and calibration, the aforementioned phenomenological elasto–viscoplasticity model for each phase of the DP steel is adapted. In this present work, the failure of DP steels is assumed to occur when the overall macroscopic stress in the softened region reaches 95% of the ultimate tensile strength (UTS). This assumption is in line with many experimental results for DP steels (e.g., see Refs. [36] and [51]). Furthermore, a void nucleation criterion is assumed when the equivalent viscoplastic strain, $\dot{\varepsilon}_\text{vp}$, reaches unity. It is important to note that a damage model should be incorporated to effectively model the ductility of DP steels. A cohesive surface model should also be utilized to model the void nucleation between the ferrite–martensite interface to accurately predict the failure of DP steels. Moreover, it is important to enhance the existing model to incorporate additional hardening due to evolution of GNDs [43,52,53]. Due to lack of sufficient experimental data to calibrate the previously mentioned models and the
complexity associated with them, such models have not been incorporated in the current work but will be the focus of future works.

For computational studies of DP steels, it is important to calibrate the constitutive model parameters of each phase based on experimental data. Several different techniques are used to determine the stress–strain response of each phase in DP steels, for example, analytical curve fitting (e.g., see Refs. [54] and [55]), X-ray diffraction (e.g., see Refs. [56] and [57]), magnetic method (e.g., Ref. [58]), and more recently microcompression pillar testing (e.g., see Ref. [36]).

Figure 2 shows the stress–strain responses of DP980 steel from two different sources: (a) microcompression pillar testing from the works of Ghassemi-Armaki et al. [36] and (b) X-ray diffraction testing from the works of Jia et al. [56]. The first set of stress–strain diagrams in Fig. 2(a) will be used to model the size-effect of the martensite particles, while the second set of stress–strain diagrams in Fig. 2(b) will be used to model the ferrite grain boundaries. It is important to mention here that the validation of these RVEs against these material properties is presented in Ref. [31].

It is noteworthy that there is no progressive softening embedded in the ferrite phase in Fig. 2(b) as compared to Fig. 2(a), but in both cases, failure is assumed at the end of the stress–strain diagram. Tables 1 and 2 show the respective calibrated material parameters for each phase that have been obtained through a regression procedure from Fig. 2.

3 Results and Discussion

3.1 Effect of Martensite Phase (Particle) Size

3.1.1 No Interphase. The first parameter that will be investigated is the effect of average size of the martensite phase. Six virtual RVEs are generated with a constant $V_{f,M}$ of 40% but with varying martensite particle sizes of 3 μm, 5 μm, and 7 μm. The first set of RVEs consists of equiaxed martensite particles, while the second set of stress–strain diagrams in Fig. 2(b) will be used to model the ferrite grain boundaries. It is important to mention here that the validation of these RVEs against these material properties is presented in Ref. [31].

It is noteworthy that there is no progressive softening embedded in the ferrite phase in Fig. 2(b) as compared to Fig. 2(a), but in both cases, failure is assumed at the end of the stress–strain diagram. Tables 1 and 2 show the respective calibrated material parameters for each phase that have been obtained through a regression procedure from Fig. 2.

### Table 1 Material parameters for individual phases of DP steels by fitting data in Fig. 2(a)

<table>
<thead>
<tr>
<th>Phase</th>
<th>$E$ (MPa)</th>
<th>$\nu$</th>
<th>$\sigma_s$ (MPa)</th>
<th>$h$ (MPa)</th>
<th>$n$</th>
<th>$m$</th>
<th>$\Gamma (1/s)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferrite phase</td>
<td>75,853</td>
<td>0.3</td>
<td>428</td>
<td>2564</td>
<td>1</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>Martensite phase</td>
<td>111,487</td>
<td>0.3</td>
<td>1918</td>
<td>8412</td>
<td>1</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>Interphase phase</td>
<td>68,313</td>
<td>0.3</td>
<td>610</td>
<td>2201</td>
<td>1</td>
<td>1</td>
<td>0.001</td>
</tr>
</tbody>
</table>

### Table 2 Material parameters for individual phases of DP steels by fitting data in Fig. 2(b)

<table>
<thead>
<tr>
<th>Phase</th>
<th>$E$ (MPa)</th>
<th>$\nu$</th>
<th>$\sigma_s$ (MPa)</th>
<th>$h$ (MPa)</th>
<th>$N$</th>
<th>$M$</th>
<th>$\Gamma (1/s)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ferrite phase</td>
<td>225,000</td>
<td>0.3</td>
<td>425</td>
<td>940</td>
<td>0.2</td>
<td>1</td>
<td>0.001</td>
</tr>
<tr>
<td>Martensite phase</td>
<td>215,000</td>
<td>0.3</td>
<td>1180</td>
<td>1740</td>
<td>1</td>
<td>1</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Figure 3 RVEs generated with a constant ferrite–martensite interphase thickness of 1 μm with varying martensite morphology of (a)–(c) equiaxed and (d)–(f) elongated. The dimension of the elongated and equiaxed RVEs are 50 × 50 μm and 100 × 100 μm, respectively.
commonly reported in many experimental results (e.g., see Refs. [2,4], and [59–61]). However, as expected, the size-effect phenomenon is not captured by these simulations. There are slight differences within the elongated RVEs; however, this is due to the interconnectivity and the distribution of the martensite phase rather than the size itself.

Figure 5 illustrates the contours of the equivalent plastic strain for different elongated martensite phase sizes without interphase. It is interesting to note that the localized plastic strains in the form of bands are evenly distributed when the martensite phase size decreases. Moreover, these bands are thicker in the RVE with 7 μm martensite phase size. However, they decrease in thickness as the martensite phase size decreases. This could be attributed to the large areas of ferrite phase between the martensite phases present in the RVE with 7 μm martensite phase size.

3.1.2 Core and Mantle Approach. As shown earlier, the classical local viscoplasticity theory is incapable of capturing size-effect [10,44,62]. However, in order to capture the size-effect of martensite phase, a strain gradient plasticity theory needs to be incorporated (e.g., see Refs. [63] and [64]). This method requires the determination of the material length scale associated with plastic strain gradient effects using some novel experiments, as well as the computational cost associated with it is very high especially when trying to simulate the currently generated RVEs [65]. Hence, this is out of the scope of this paper and will be addressed in a future work. However, another simple way of capturing martensite size-effect is through introducing an interphase between martensite and ferrite regions to account for the GNDs stored within this interphase [31]. This method is called the core and mantle approach [41] and is much simpler than the strain gradient plasticity theory approach. For simplicity, the core and mantle approach is adopted here in order to capture size-effect of martensite phase.

The same RVEs in Fig. 3 are simulated, but this time an interphase of 1 μm thickness is assumed at the ferrite–martensite interphase [36]. The overall stress–strain responses are shown in Fig. 4(b). As for the equiaxed RVE, the results show that this method is capable of capturing the size-effect phenomenon, where smaller is stronger. However, as for the elongated RVEs, the results do not show a clear trend. Interestingly, the ductility is increasing as the martensite phase size decreases; however, the UTS is roughly the same for all three elongated RVEs. The reason why a clear size-effect phenomenon was not seen is because both distribution and interconnectivity of martensite particles also play a role on the overall response of DP steel, which in this case (elongated RVEs) is not kept constant [5]. Hence, these two morphological parameters besides size-effect contribute to the overall stress–strain behavior.

It is important to mention here that the martensite phase size does play a role in the overall behavior. In a study by Erdogan and Tekeli [66], it was shown, through experiments, that as the martensite phase size decreases, the strength and the ductility increase simultaneously. This experimental observation agrees with the simulation results from the equiaxed RVEs. Hence, it can be concluded that the core and mantle approach can capture size-effect as well as the martensite morphology effect.
Figure 6 shows the contours of equivalent plastic strain for the core and mantle model. Interestingly, the strain localization in the form of localized bands looks similar to that presented in Fig. 5. Similarly, the distribution of localized bands is more in the RVE with smaller martensite particle size. In Sec. 3.2, the effect of ferrite grain size and boundary will be discussed.

3.2 Effect of Ferrite Grains

3.2.1 Effect of Ferrite Grain Size. In this section, the effect of ferrite grain size will be discussed. It is noteworthy that this paper will not model the grains of the martensite phase, as this phase is significantly stronger than the ferrite phase. Hence, it is expected that the grains in the martensite phase will not affect the overall response. Here, six virtual RVEs are generated with a constant \( V_{f,M} \) of 40%. The first three RVEs are modeled with elongated martensite phase (AR = 10), while the last three RVEs are modeled with equiaxed martensite phase (AR = 1). Both these sets of RVEs consist of varying grain sizes of 7 \( \mu \)m, 5 \( \mu \)m, and 2 \( \mu \)m. Figure 7 shows these RVEs.

As in Sec. 3.1, the methodology that is used to model the grain boundaries is the core and mantle method [41]. In this method, the grain boundaries are modeled by placing a finite layer or an interphase along the grain boundaries. The material properties that have been assumed for the grain boundary consist of a very high yield strength such that no grain boundary yielding occurs, which represents the case of a hard boundary where dislocations are not allowed to transfer through the boundary. This is a commonly adapted assumption that is used for modeling grain boundaries (e.g., see Refs. [52] and [67]). Furthermore, for simplicity, there is no grain boundary sliding/deboning considered in this work. It is important to note that due to the lack of available experimental data, it is very difficult to calibrate such boundary-based constitutive models; hence, a hard boundary assumption is taken for this study.

Figure 8 shows the corresponding stress–strain responses of the RVEs in Fig. 7. As commonly observed [6,68,69], the results show that the strength increases with the decrease of grain size on the expense of ductility. But more importantly, all the RVEs with elongated martensite phase consist of higher strength and ductility as compared to their respective equiaxed RVEs (see Fig. 9). It is interesting to note that the rate of change in the UTS and yield strength is the same with respect to grain size. The change in ductility (strain level at 95% UTS) is more drastic for elongated RVEs (with AR = 10) as compared to equiaxed RVEs (with AR = 1). Moreover, the strain level at UTS is unaffected by the grain size for the case of equiaxed martensite particles. In Sec. 3.2.2, the effect of elongated ferrite grains (i.e., grain morphology) will be discussed.

3.2.2 Effect of Elongated Versus Equiaxed Ferrite Grains. In this section, the effect of elongated grains on the overall stress–strain behavior of DP steel with equiaxed and elongated
martensite phase will be explored. Six RVEs were generated with constant 40% $V_f,M$ while varying the AR of the ferrite grains to 1, 5, and 10. The first three RVEs are with equiaxed martensite phase (AR = 1), while the last three RVEs are with elongated martensite phase (AR = 10). These RVEs are presented in Fig. 10. The RVEs are loaded in the horizontal (x-direction) or vertical (y-direction) directions. Figure 11(a) shows the stress–strain responses for the equiaxed martensite phase, while Fig. 11(b) shows the results for the elongated martensite phase. These figures also show the results in case ferrite grains are not considered (i.e., the grainless case). It is seen that as the grains are elongated or stretched along the loading direction, both the yield strength and UTS increase on the expense of ductility for both equiaxed and elongated RVEs. In fact, this trend is parallel to the trend observed when decreasing the grain size, but opposite to what have been noticed when the martensite particles are elongated (see Fig. 4(a)). Moreover, the results again show that DP steel with elongated martensite phase has superior properties with respect to DP steel with equiaxed martensite phase.

The same figures also demonstrate the behavior of these RVEs when the loading is in the y-direction (i.e., perpendicular to elongation axis). In the RVEs of equiaxed martensite, the stress–strain response of both the RVEs with grain’s AR of 5 and 10 are the same as of the RVE with grain’s AR of 1 when the loading is applied in the y-direction (i.e., the overall response in the y-direction is independent of the grain’s aspect ratio). It is worth mentioning that the thickness of the grains in the y-direction decreases as the AR increases; however, this has little impact on the overall response when the load is applied in the y-direction. In the case of equiaxed martensite phase, the change in stress–strain response is only due to the grain boundaries when the direction of loading changes.

Moreover, the RVEs with elongated martensite phase were also loaded in the y-direction and their responses are shown in Fig. 11(b). Unlike the equiaxed martensite RVEs, the common trend of increase in strength on the expense of ductility is seen as the AR of the grains increases when the loading is applied in the y-direction; the increase in UTS is not significant as compared to
the decrease in ductility. There is a significant difference in the stress–strain response of the elongated RVEs with a grain’s AR of 5 and 10 when the load is applied in the y-direction as compared to the loading in the x-direction. But overall, it is confirmed, through these results, that an RVE with elongated grains exhibits anisotropic behavior.

4 Conclusions

This paper focuses on exploring the effect of size and morphology of martensite particles and ferrite grains on the overall mechanical behavior of DP steels. As for the martensite particle size, it is shown that the local viscoplasticity theory is incapable of capturing size-effect; hence, the core and mantle approach, which assumes the existence of a thin interface of GNDs between the ferrite and martensite phases, is adopted which is shown that it can capture martensite particle and ferrite grain size-effects if all the other microstructural parameters are kept constant.

For the same ferrite grain size, it is clearly shown for DP steels with equiaxed martensite particles that as martensite particle size decreases, the yield strength, UTS, and ductility are increased simultaneously. Moreover, for the same ferrite grain size, elongating the martensite particles along the loading direction increases yield strength, UTS, and ductility simultaneously. On the other hand, increasing the ferrite grain size decreases while fixing the aspect ratio of the martensite particles, the overall UTS increases on expense of the ductility. However, the decrease in ductility with decreasing ferrite grain size for the equiaxed martensite particles is not as significant for elongated martensite particles. Likewise, as the aspect ratio of the ferrite grains increases, similar behavior is seen. When the loading is applied perpendicular to the elongation direction of the ferrite grains, the aspect ratio of the ferrite grains does not affect the results much for the case of equiaxed martensite particles; however, decrease in ductility is seen for the case of elongated martensite particles. It is obvious from this study that decreasing the martensite size and increasing its aspect ratio along the loading direction while fixing the grain size might be more efficient in the simultaneous increase in strength and ductility of DP steels.

References


