Computational modeling of the effect of equiaxed heterogeneous microstructures on strength and ductility of dual phase steels

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In this study, a code was developed to create virtual random representative volume elements (RVEs) depicting the actual and highly equiaxed heterogeneous microstructure of ferrite–martensite dual phase (DP) steels. Within this approach it was possible to perform a parametric study of the effects of DP microstructure (e.g., volume fraction, size, and distribution of the martensite; grain size and boundaries of the ferrite; martensite–ferrite interphase) and mechanical properties of the ferrite and martensite phases on the overall stress–strain behavior. A finite strain elastic–viscoplastic constitutive model has been used in conducting these microstructural-based simulations. It is shown that plastic strain localization in the form of localized narrow bands significantly control the ductility and ultimate fracture of DP steels. It was also noticed that by adding viscosity into the material property, the ductility increased significantly without compromising the strength of DP steels. It is shown that by decreasing the size of martensite phase and considering the ferrite–martensite interphase the overall response yields a simultaneous increase in strength and ductility.

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1. Introduction

Dual phase (DP) steel is a type of advanced high strength steel (AHSS) which consists of two main phases distributed heterogeneously within the microstructure [74]. It is widely used in the automotive industries because of its high strength to weight and low yield to ultimate strength ratios and low manufacturing cost [51]. These steels consist primary of hard martensite phases embedded into a softer ferrite matrix phase. They may sometimes include bainitic phases as well [59]. It is well-known that the mechanical properties of DP steel depend on its grain size, volume fraction, morphology (elongated or equiaxed), and carbon content of each phase (e.g., [28,50,64,79]). Throughout this paper, our discussion will be focused only on DP steels consisting of martensite and ferrite phases where the morphology of the martensite phase will be equiaxed (i.e., martensite islands that have axes of approximately the same length).

In the last decade, there has been a significant increase of interest on exploring ways of improving the mechanical performance of AHSS through microstructural computational modeling of representative volume element (RVE). In the early works of Al-Abbas and Nemes [6–8], micromechanical simulations were conducted on DP steels that were idealized to be spherical inclusions of martensite embedded in the ferrite matrix. These papers were followed by a series of papers by Khaleel and his co-workers (e.g., [19,20,82,83]) in which they used the classical (local) plasticity theory on RVEs generated from real scanning electron microscope (SEM). It was concluded from their works, that the failure of DP steels is driven by softening and failure due to plastic strain localization rather than nucleation, coalescence, and growth of voids. The aforementioned studies have been followed by a series of papers by Ramazani and his co-workers [66,68,69,70–73] that contributed a significant effort in understanding the behavior of DP steels through RVE-based computational modeling. The failure mode of DP steels using the Gurson–Tvergaard–Needleman (GTN) model [66] and extended finite element method (XFEM) [67,73] were studied. Moreover, the effect of bainite phase within the DP steel was also investigated [72]. It was shown that with the presence of bainite, the internal stress gradient was reduced while the overall strength was increased. Further, the effect of banding or elongating the martensite within the DP steel was also investigated [67,68]. It was shown that the yield strength decreases as the aspect ratio of the banded martensite increases.

Further, several works were performed in which various RVE-based microstructures were used to simulate plastic flow behavior of DP steels (e.g., [18,21,47,48,49,55,61,80,87]).
Despite the above mentioned work, it is highly desirable to adopt methods as accurate as possible to explore the relationship between the microstructure and the corresponding overall behavior of DP steels. There are key challenges that still remain in this research field which this paper tries to overcome. For example, mesh sensitivity is an unresolved issue in modeling DP steels. This is because all of the aforementioned papers are using the classical (local) rate-independent plasticity theory or local plasticity-damage theory and it is well-known that these theories exhibit mesh-dependent results while modeling plastic strain localization or localized damage/fracture (e.g., [3,4,12,25,27]). The issue of mesh sensitivity is very critical as it makes it difficult to correctly predict the strength and ductility of DP steels. One possible solution to this problem is the involvement of a higher-order gradient-dependent plasticity model (e.g., [3,4,24,94]). However, the numerical implementation and computational cost of the non-local theories for conducting complex finite element simulations is costly [24,27,31]. Therefore, in this paper a simple technique based on viscosity regularization will be used to get mesh-independent results (e.g., [26,56,91]). The use of gradient-dependent plasticity theory will be explored in future work.

Another important challenge in micromechanical modeling of DP steel is mimicking the actual microstructure. There are several techniques found in literature that have been used to generate microstructures of DP steels that can be categorized into two approaches: (1) artificial microstructures and (2) microscopy-based real microstructures. As for the artificial microstructures, checker-box (e.g., [60,70,86,87]), circles (e.g., [9,11,47]), and the well-known Voronoi tessellation (e.g., [39,40,58]) have been used. In these methods, plastic strain localization is significantly influenced by the unrealistic geometry of the martensitic islands. As for generating real microstructures, scanning electron microscope (SEM) images (e.g., [19,41,48,67,69,83]) and electron backscatter diffraction (EBSD) [72,73,76] have been used. Despite the fact that these microscopy-based RVEs preserve the complexity of the microstructure, it limits the user's ability to vary the microstructure. More recently, in the works of Madej et al. [53] the method of using digital material representation (DMR) to generate microstructures of DP steels was introduced. In this method, SEM images combined with Voronoi tessellation are used to generate virtual RVEs. One of the prime focuses of this paper is to present a new method of generating virtual RVEs which gives the user full

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![Fig. 1. Schematic diagram for generating virtual RVEs of DP steels.](image-url)
The ability to control its parameters while keeping the DP microstructure as real as possible.

It was shown in the work of Kadkhodapour et al. [47], who used nano-indentation, that the ferrite phase plastically behaves inhomogeneously. This is primarily due to the presence of geometrically necessary dislocations (GNDs) at the interphase of the two phases. However, most of the aforementioned works have not taken this into account. Moreover, Kadkhodapour et al. [47] and Ramazani et al. [69] 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 micro-compression pillar testing that was performed by Ghassemi-Armaki et al. [37].

Another important parameter in micromechanical modeling of DP steels is the grain size of the ferrite phase [62]. It was shown recently in the work of Calcagnotto et al. [15] that the yield strength and the tensile strength 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 the increasing the GNDs along the ferrite and martensite boundaries [46]. There are many methods proposed in literature for modeling the grain size effect. The most commonly used is the well-known Hall–Petch relationship [63], which is based on dislocation 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., [34,35]), 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., [2,6,59,92]). For simplicity, in this paper, the “core and mantle” approach is used to incorporate the grain size effect on the overall response of DP steels. The same approach is also employed to incorporate the martensite phase (particle) size effect.

The objectives of this paper are as follows: (1) an improved approach in mimicking the actual microstructure of DP steels through virtual material design is presented. The microstructures generated through this method, not only look similar to the actual SEM images but also behave similarly under mechanical loading conditions. (2) A simple approach in eliminating the finite element mesh sensitivity through viscosity regulation is adapted. (3) A parametric study is conducted on the effects of various microstructural parameters (e.g., martensite size, distribution, and volume fraction, ferrite grain size and grain boundary, interface between the martensite and ferrite) on the overall stress–strain response and plastic strain localization patterns.

2. DP microstructural modeling

2.1. Virtual RVE generation

In this section, the microstructural finite element modeling of DP steels is presented. As for the microstructure, a code was developed in Matlab for generating random two-dimensional (2D) RVEs. The generation of the virtual RVEs is based on the Voronoi’s tessellation [89]; however, modified to obtain more accurate DP microstructures. Voronoi tessellations have been used to generate the microstructure of various types of steels (e.g., [14,38,39,40,48,52,57]).

The Matlab code that is developed in this study utilizes the inbuilt Voronoi tessellation function within the Matlab database. The code supplies the coordinates of the randomly distributed seeds to the Voronoi tessellation function while this function provides back to the code the coordinates of the generated tessellation cells and their connectivity. Once this data has been obtained, the code uses an optimization and filtering algorithms to generate a microstructure based on the desired geometric parameters (e.g., volume fraction, minimum and maximum size, morphology, and
distribution) for the martensite phase. This is illustrated in Fig. 1. To generate the grain boundaries within the existing microstructure, the code returns back to the Voronoi tessellation function a new set of randomly distributed seeds. The Voronoi tessellation function then produces a new set of Voronoi cells and gives the code the coordinates along with its connectivity. This is patched onto the existing microstructure without any modification. Once the RVE is finalized in Matlab, a STereoLithography (stl) file is created. This file is then transferred to SolidWorks software where it is converted into a drawing file which can be easily imported into Abaqus finite element software. As compared to other Voronoi tessellations that have been adapted in the literature, the current code incorporates also: (1) a post-Voronoi algorithm which enhances the microstructure by controlling the size distribution and morphology of the martensite phase, (2) the grain size distribution for the ferrite phase, (3) the flexibility of adding several other phases, and (4) independent meshing within the finite element software.

For example, two virtual RVEs are presented in Fig. 2 and compared with real SEM based RVEs attained from the work of Sun et al. [83]. The virtual and SEM based RVEs possess the same volume fraction of martensite ($V_{(M)}$). Generally, the morphology of martensitic phase in DP steel can be categorized as equiaxed (equal-axes), elongated in certain direction, or a combination of both [64]. Note that the actual microstructure in Fig. 2(c) and (d) show a combination of both equiaxed and short elongated martensite islands. However, the focus of the current paper is on virtually generating and computationally modeling the equiaxed morphology as shown in Fig. 2(a) and (b).

It is important to perform a statistical distribution analysis on the virtual RVEs to understand the distribution process of the code. Fig. 3 shows an analysis conducted on the virtual RVE presented in Fig. 2(a). Each martensite particle is analyzed for its dimensions in the x- and y-axes along with its area. Note from Fig. 3(a), (c), and (e) that the majority of the results for each parameter are clustered with a small deviation. This is further clarified in Fig. 3(b) and (d).

![Fig. 3. Statistical size distribution of RVE presented in Fig. 2(a) for: (a) and (b) size in x-direction, (c) and (d) size in y-direction, (e) area, and (f) comparing 10 different RVEs with constant equiaxed martensite volume fractions.](image-url)
where a log-normal size distribution is obtained. In Matlab, there are several methods of producing randomly distributed seeds within a specific domain. Here, a uniform distribution of initial seeds for the Voronoi tessellation is assumed, which results in equiaxed microstructure such that different random distributions of the martensite particles may not change the martensite particle size distribution. This is clearer in Fig. 3(f) where ten RVEs were generated with the same martensite volume fraction to analyze the average particle size in the $x$- and $y$-directions along with the corresponding area. Note that despite the difference in the distribution, the average $x$-and $y$-distance along with the area do not change from one RVE to another. Hence, it is anticipated that for these microstructures, statistical distribution of the martensite particles within the RVE is not a parameter that will influence the results. This becomes clearer in Section 3.3 where the effect of distribution on the overall behavior is discussed.

Several researchers have compared 2D modeling with 3D modeling of DP steels (e.g., [16,70,72,76]). All of them have concluded that the computational cost increases significantly when dealing with 3D simulations. Moreover, in the works of Ramazani et al. [72] it was shown that the stress–strain responses from 2D and 3D RVEs are comparable. Therefore, in the current paper, 2D RVEs are generated and simulated.

In the present paper, it is assumed that there is perfect bonding between the two phases during the entire deformation process. DP steels are generally manufactured as thin sheet specimens where the $x$- and $y$-directions are relatively larger than the $z$-direction. Taking this into consideration, the microstructure presented in this paper is assumed to be under the plane-stress state.

RVE size is an important parameter which influences the computational simulation results. For example, Ramazani et al. [68] showed that the minimum size of a DP steel RVE is 24 $\mu$m with at least 19 equiaxed-martensite grains, while Asgari et al. [11] determined that 10 $\mu$m is a proper RVE size for modeling DP steels. However, it is imperative that the volume fraction of the martensite phase is maintained constant when investigating the effect of the RVE size, which is not straightforward when using RVEs from real microstructures as compared to RVEs from virtual microstructures. By conducting a convergence study, where the volume fraction of the martensite phase is maintained constant, it was found an RVE size of 100 $\mu$m is sufficient to get converged results. However, this is also dependent on the imposed boundary conditions on the RVE. In fact, it is concluded by several studies that periodic boundary conditions (e.g., [5,36,44,45]) yield the proper size of the RVE and the most accurate results. Therefore, periodic boundary conditions are imposed here.

The boundary conditions applied on the 2D microstructures are the following. The left-edge of the RVEs is fixed in the $x$-direction, but is free to move in the $y$-direction. The bottom-edge of the RVEs is fixed in the $y$-direction, but is free to move in the $x$-direction. The top-edge of the RVEs is free to move in the $x$-direction but will move synchronizingly in the $y$-direction to preserve the compatibility with adjacent bodies (i.e., periodicity). The right-edge of the RVEs is under displacement-controlled tensile loading in the $x$-direction. These boundary conditions have been used throughout this study. As for the mesh size, this will be discussed in detail in the next section.

### Table 1

<table>
<thead>
<tr>
<th>Material parameters for individual phases of DP steels.</th>
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<tr>
<td><strong>Ferrite phase</strong></td>
</tr>
<tr>
<td>$E$ (MPa)</td>
</tr>
<tr>
<td>$\nu$</td>
</tr>
<tr>
<td>$\sigma_y$ (MPa)</td>
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<tr>
<td>$h$ (MPa)</td>
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<td>$n$</td>
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<td>$m$</td>
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<td>$\Gamma$ (1/s)</td>
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2.2. Finite deformation elastic–viscoplastic constitutive model

The commercial finite element code Abaqus [1] was used for this study. Each phase in the DP steel is modeled as a finite deformation elastic–viscoplastic material and modeled using von Mises plasticity. The total rate of deformation tensor, $\mathbf{D}$, is additively decomposed as follows:

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

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

$$\dot{\mathbf{\sigma}} = \frac{E}{(1 + \nu)} \left[ \mathbf{D}^e + \frac{\nu}{(1 - 2\nu)} \mathbf{D}^{\text{el}} \right]$$

where $E$ is the Young’s modulus, $\nu$ is the Poisson’s ratio, and $\mathbf{I}$ is the second-order identity tensor.

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

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

with

$$\dot{\varepsilon}_{\text{vp}} = \sqrt{\frac{2}{3}} \mathbf{S} : \mathbf{S}$$

and

$$\mathbf{S} = \mathbf{\sigma} - \frac{1}{3} \mathbf{\sigma} \mathbf{I}$$

(3)

and

$$\dot{\varepsilon}_{\text{vp}} = \Gamma \left( \frac{\sigma_y}{h} - 1 \right)^{\frac{1}{n}}$$

(4)

where $\sigma_y$ is the yield strength, $\Gamma$ is the inverse of the relaxation time, which is a fluidity parameter or the inverse of the viscosity parameter, $h$ is the hardening modulus, and $\langle \rangle$ is the Macaulay bracket. The equivalent viscoplastic strain $\dot{\varepsilon}_{\text{vp}}$ is defined as

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

It is noteworthy that a more physically-based model such as the dislocation density-based model [75] or the crystal plasticity model [22] is not adapted in this work because of the high computational cost and complexity associated with such models.
especially in modeling the complicated microstructures of DP steels. Also, there are many material parameters associated with these models that need to be calibrated for each phase in the DP steel, which is not an easy task based on the very limited experimental data for each phase. Therefore, for simplicity and for reducing the computational cost, we adapted the phenomenological elasto-viscoplasticity theory for modeling each phase which is also much easier to calibrate.

In this work, it is assumed that failure of the DP steel occurs when the estimated overall macroscopic stress in the softening part of the stress–strain diagram reaches 95% of the predicted ultimate tensile strength (UTS). In fact, this assumption is supported by many of the experimental data that have been obtained for DP steels (e.g., [23,37,77]). Moreover, void nucleation is assumed to occur when the equivalent plastic strain, $e_{vp}$, reaches unity. However, it should be emphasized that a damage model should be employed in order to effectively simulate the void evolution and crack propagation within each phase that lead to ultimate failure of the DP steel. A cohesive surface model should be used to effectively simulate void nucleation at the ferrite–martensite interface in order to more effectively predict the ultimate failure of the DP steel. Further, the current constitutive model should be enhanced through incorporating plastic strain gradients which allows one to more accurately incorporate additional hardening due to evolution of geometrically necessary dislocations (e.g., [2,10,32]). Unfortunately, due to the lack of sufficient experimental data that can be used to effectively formulate and calibrate such damage, cohesive surface, and strain gradient plasticity models, these models are not adapted in the current study and should be the focus of future work.

2.3. Phase material parameters

For computational modeling of DP steels, it is crucial to determine the material properties of each individual phases. There are many techniques that have been proposed in literature for this purpose. X-ray diffraction [43,93], analytical curve fitting [54,84] and magnetic method [65] are some techniques used for this purpose. The results from these techniques can differ due to the limitations that may exist in each method. Due to the advancement of technology at the nano level, it has been possible to perform nanoindentation and micropillar compression testing for each phases of DP steel and at close proximity of boundary of each phase [37].
The stress–strain responses of martensite and ferrite phases of DP980 are presented in Fig. 4 [43]. Based on regression procedure the material parameters for each phase are obtained and presented in Table 1. It is noteworthy that there is softening embedded into the ferrite phase when the stress–strain response is plotted in the engineering stress–engineering strain space (see Fig. 4). Also, Abaqus assumes that the material has failed at the last point in the assigned true stress–strain response. These parameters will be used throughout the paper, unless specified otherwise.

3. Results and discussion

3.1. Analysis of mesh-size dependency

A common challenge that is faced in simulating plastic strain localization within the microstructure of the DP steel through using the classical local constitutive model is that the results are mesh-size dependent. This is because the finite element solution does not converge with an increase in the mesh density. More details are mentioned in Section 1.
Sun et al. [82] performed a mesh sensitivity study on microstructural modeling of DP steels and found that the results are mesh-dependent. It was observed that by using a coarse mesh at the ferrite grain boundary, a stronger stress–strain response was found as compared to a finer mesh. This is because a finer mesh accelerates the localization such that it fails quicker with a high steep post-critical slope as compared to a coarser mesh [78].

In this study, mesh sensitivity analysis is performed on one of the virtual RVEs with 40% \( V_{\text{f,M}} \) as shown in Fig. 5. The RVE is initially generated in Matlab and then transferred to Abaqus where the RVE is meshed and the boundary conditions are applied. Plane stress quadratic elements with reduced integration (CPS4R) were selected for this study. The applied strain rate is \( 10^{-3} \) s\(^{-1}\). Also, as stated in Section 2.2, micro-voids are assumed to nucleate when the equivalent viscoplastic strain reaches one, whereas failure of the RVE is assumed to occur when the macroscopic stress in the softening part of the calculated stress–strain diagram reaches 95% of the ultimate strength. The results of the mesh sensitivity are presented in Figs. 6 and 7. It is evident from Fig. 6 that the obtained macroscopic stress–strain response is mesh-dependent. In order to resolve the mesh sensitivity issue two physically unsound approaches are found in literature when modeling the microstructure of DP steels; namely, by comparing with experimental results to find the correct mesh size (e.g. [82]) and through using a constant mesh size (e.g. [60]).

In this paper, the viscosity-type regularization is used to overcome the mesh-dependency through the use of the viscoplasticity model presented in Section 2.2 [26,56,91]. Small controlled amount of viscosity has been added to both the martensite and ferrite properties such that the behavior of both phases does not change significantly. Though, this approach induces rate-dependent phases. With this viscosity regulation, the results become much less dependent on mesh size as shown in Figs. 6 and 7. However, one can see a clear convergence of the results as the mesh density is increased. This method is simple and does not increase the computational cost. However, with the use of a viscosity parameter (i.e., making each phase slightly rate-dependent) an interesting behavior is attained where the overall ductility of the material increases significantly while the ultimate tensile strength (UTS) does not change when compared with the results without viscosity-based regularization. This interesting behavior, which can be enhanced through dispersion of hard viscoelastic second-phase particles within the microstructure of DP steel, will be explored further in future work.

Figs. 8 and 9 compare the failure modes of both cases, without and with viscosity-type regularization. It is evident that plastic strain localization in the form of narrow shear bands is formed, where the density of these shear bands increases as loading increases. The shear bands are more intense and distributed within the microstructure of the RVE when the viscosity regularization is applied. This might be the reason why the ductility is increased with viscosity. Fig. 9 shows the distribution of the equivalent plastic strain at 95% of UTS. This clearly shows that failure occurs within few localized regions for the case without viscosity while failure occurs within many localized regions for the case with viscosity.

3.2. Comparing results from SEM-based and virtual RVEs

For validation of the results from the current virtual RVEs, the SEM-based and corresponding virtual RVEs of 15% and 38% \( V_{\text{f,M}} \) as shown in Fig. 2 are simulated. The results are compared in (b). Fig. 10 shows that one can get an agreement with the corresponding experimental response for a certain FE mesh density when viscoplasticity is not taken into consideration (i.e., rate-independent plasticity is used), which is physically not sound as the results are mesh sensitive. This was discussed in detail in the previous section. However, when using viscoplasticity (i.e., rate-dependent plasticity), mesh-independent results are obtained that match well the measured ultimate tensile strength but not the ductility. Therefore, adding viscosity effect to the constitutive behavior significantly overestimates the ductility as compared to experimental measurements. On the other hand, the results from the SEM-based RVEs and the virtual RVEs are quite similar with little discrepancy when using the viscoplasticity model for simulating both RVEs. The reason for this discrepancy is due to the effect of morphology which plays a key role in the overall behavior [79].

It is important to mention that all the results, with viscosity (i.e., when using the viscoplastic model) and without viscosity (i.e., using the rate-independent plasticity), yield the same UTS and the yield strength while differing in the ductility. The reason why the ductility increases with the addition of viscosity effect is because of the nature of rate-dependent materials. It is known that globally the strain-rate is the same as the one defined by the user which is assumed to be quasi-static in this paper. However, locally the strain-rate might increases in certain areas within the RVE which activates the rate-effect hence causing the overall ductility to increase significantly. This phenomenon will be explored deeply by the authors in the future. Nevertheless, Fig. 10 demonstrates the ability of the virtually generated RVEs to predict the overall behavior of DP steels.

The results reflect accurate prediction of the UTS and its corresponding strain for both RVEs. The difference in the UTS between the SEM-based RVE and the virtual RVE is only 7 MPa.

![Fig. 10. Comparing the stress–strain results from SEM-based RVE and virtual RVE for 15% and 38% \( V_{\text{f,M}} \).](image)
Moreover, the difference in the corresponding strain at UTS for both RVEs is only 0.05% and 0.55% for 15% and 38% $V_{f,M}$, respectively. As for the strain at 95% of UTS, the results show slight discrepancy. One reason why the differences do show up is because of the morphology of the martensite islands. The SEM-based RVEs consist of both equiaxed and elongated martensite islands; however, this is not the case for the virtual RVEs with equiaxed islands only. The effect of the martensite morphology will be investigated in future work. Nevertheless, the difference is quite small and hence, this method of creating virtual RVEs is proven to show acceptable results.

Fig. 11 shows the distribution of the equivalent plastic strain for the SEM-based RVE, SEM image shown in Fig. 2(b) and a virtual RVE, shown in Fig. 2(a), at various engineering strain levels of (a) 5%, (b) 11.6% (SEM based RVE, and 11% (virtual RVE), (c) 24.8% (SEM based RVE), and 22.9% (virtual RVE)) ($V_{f,M} = 15\%$).

Fig. 12. Virtual RVEs at constant $V_{f,M}$ off 30% with random distributions: (a) RVE-1, (b) RVE-2, (c) RVE-3, and (d) RVE-4.

for 15% $V_{f,M}$ and 6 MPa for 38% $V_{f,M}$. Moreover, the difference in the corresponding strain at UTS for both RVEs is only 0.05% and 0.55% for 15% and 38% $V_{f,M}$, respectively. As for the strain at 95% of UTS, the results show slight discrepancy. One reason why the differences do show up is because of the morphology of the martensite islands. The SEM-based RVEs consist of both equiaxed and elongated martensite islands; however, this is not the case for the virtual RVEs with equiaxed islands only. The effect of the martensite morphology will be investigated in future work. Nevertheless, the difference is quite small and hence, this method of creating virtual RVEs is proven to show acceptable results.

Fig. 11 shows the distribution of the equivalent plastic strain for the SEM-based RVE and the virtual RVE at 95% of UTS for 15% $V_{f,M}$. Although crack propagation and void nucleation are not modeled explicitly, Fig. 11 clearly shows the shear bands and crack propagation along the localized zones. Also, in Fig. 11(c), there

![Fig. 11. Distribution of equivalent plastic strain of SEM-based RVE, SEM image shown in Fig. 2(b) and a virtual RVE, shown in Fig. 2(a), at various engineering strain levels of (a) 5%, (b) 11.6% (SEM based RVE, and 11% (virtual RVE), (c) 24.8% (SEM based RVE), and 22.9% (virtual RVE)) ($V_{f,M} = 15\%$).](image)

![Fig. 12. Virtual RVEs at constant $V_{f,M}$ off 30% with random distributions: (a) RVE-1, (b) RVE-2, (c) RVE-3, and (d) RVE-4.](image)

![Fig. 13. Macroscopic responses of the RVEs, shown in Fig. 12, under uniaxial tension.](image)
are numerous micro-voids that are nucleated at the boundaries of the martensite phase.

3.3. Effect of martensite microstructural distribution

This section focuses on studying the effect of random distribution of the martensite phase within the microstructure on the overall stress–strain response of DP steels. Four virtual RVEs with 30\% V_{f,M} are generated with random distributions of the martensite phase as shown in Fig. 12. It is important to highlight here that the statistical distribution within the RVE was discussed in Section 2.1; however, here we will investigate the effect of the martensite distribution of equiaxed morphology on the DP overall stress–strain response.

Fig. 14. Distribution of equivalent plastic strain of RVEs, shown in Fig. 12, at various average strain levels of (a) 4\%, (b) at tensile strength (strain: 9.7\% (RVE-1), 9.5\% (RVE-2), 9.4\% (RVE-3), and 10.1\% (RVE-4)), and (c) at 95\% of tensile strength (strain: 19.8\% (RVE-1), 19.6\% (RVE-2), 19.3\% (RVE-3), and 19.8\% (RVE-4)).

Fig. 15. Virtual RVEs generated at different volume fraction of martensite of (a) 20\%, (b) 30\%, (c) 40\%, (d) 50\%, and (e) 60\%. 
The macroscopic stress–strain responses for all the four RVEs are shown in Fig. 13. It is clear from the results that the arrangement of martensite phase has no influence on the stress–strain curve. This is true for the case of an equiaxed martensite phase. The results may change significantly when the morphology of the martensite phase is elongated in a certain direction, which will be investigated in future work.

Fig. 14 shows the distribution of equivalent plastic strain of all RVEs at different strain levels. Multiple shear bands and small voids are visible in all the cases. There is slight deformation in the martensite phase. This is due to their superior mechanical properties compared to ferrite. Furthermore, it is clear that the crack propagation and shear band thickness are influenced by the arrangements of martensite phase; however, the overall response is not affected.

3.4. Effect of volume fraction of martensite

The martensite volume fraction \( V_{\text{f,M}} \), is a key factor which influences the strength and ductility of DP steels. Martensite, being a hard material, dominates when its volume fraction is increased. In this section, five RVEs are generated with different \( V_{\text{f,M}} \) ranging from 20% to 60% as shown in Fig. 15. The corresponding results are presented in Fig. 16. As expected and commonly reported (e.g., \([42,62]\)) as \( V_{\text{f,M}} \) increases, the overall strength of the material increases; however, this comes with the compromise of ductility (see Figs. 16 and 17).

Fig. 18 shows the equivalent plastic strain distribution at different strain levels. It can be seen that the shear bands are thicker and more intense for the 20% \( V_{\text{f,M}} \) as compared to other volume fractions. This is primarily due to the low \( V_{\text{f,M}} \) and the large spacing between the martensite islands. Furthermore, small voids are found along the shear bands in the ferrite phase for all the RVEs. These voids will grow within the localized plastic regions and are the reason for the final failure of the material along the localized zones.

3.5. Effect of martensite phase (particle) size

Another parameter that is studied is the average size of the martensite phase. Three virtual RVEs are generated with a constant \( V_{\text{f,M}} \) of 40% but with different sizes of the martensite phase (3 \( \mu m \), 5 \( \mu m \), and 7 \( \mu m \)) as shown in Fig. 19. It is worth mentioning that the average size of the martensite phase was measured based on the average size of each particle in the \( x- \) and \( y- \)directions as was demonstrated in Fig. 3.

Fig. 20 shows the stress–strain responses of all the three RVEs. It is evident from the figure that the size does not affect the yield strength and UTS. The ductility, on the other hand, is varying slightly. This variation in ductility is related to the evolution of the localized plastic zones within the microstructure of the DP steel which is governed by the refined distribution of the martensite as its size decreases. Fig. 21, on the other hand, shows the distribution of the equivalent plastic strain at different strain levels. It is seen that the RVE with the smallest martensite island size has more intense distribution of plastic shear bands. On the other hand, the RVE with the largest martensite islands has thicker shear bands.

It is noteworthy to mention that the classical local plasticity theory is not capable of capturing size effect (e.g., \([7,59,90]\)); hence, a gradient plasticity theory needs to be incorporated in order to capture the size effect of the martensite phase. This will be addressed in future work. However, another approach that can be used to capture this size effect is through introducing an interphase between the martensite and ferrite phases where geometrically necessary dislocations (GNDs) are localized. This interphase has stronger properties than that of ferrite. This will be shown in the following subsection using the so-called “core and mantle” hardening model (e.g., \([34,35]\)) in which the phase boundaries are modeled by placing a thin layer or an interphase of finite thickness along the grain boundaries. In this work, effects of GNDs in close proximity of ferrite grain boundaries and ferrite–martensite boundaries on the overall behavior of the DP steel is implicitly incorporated through adding the interphase at these boundaries with different mechanical properties. This is a much simpler approach than the gradient plasticity theory where the evolution of GNDs is incorporated explicitly (e.g., \([2,10,59,59]\)).

3.6. Effect of ferrite–martensite interphase

In this section, the effect of interphase between martensite and ferrite where GNDs are stored is studied. A common assumption that is taken while preforming microstructural modeling of DP steels is that the ferrite properties are homogeneous throughout the ferrite phase (e.g., \([19,82,83]\)); however, this is not the case in reality. In fact, a study using nanoindentation and micro-pillar compression testing showed that the mechanical properties of ferrite are different near the martensite phase \([37,47]\).

For this study, the material properties for ferrite, martensite, and interphase are obtained from the works of Ghassemi-Armaki et al. \([37]\); in which nano-compression pillar testing was performed on DP steels (see Fig. 22). It is noteworthy that there is no progressive softening seen in the stress–strain response of each phase as compared to Fig. 4, but in the simulations failure of each phase is assumed at the end of the stress–strain diagram.

![Fig. 16. Macroscopic responses of RVEs with varying martensite volume fraction.](image)

![Fig. 17. Tensile strength, strain at tensile strength, and strain at 95% tensile strength as a function of volume fraction of martensite.](image)
Based on regression procedure the material parameters for each phase are obtained and presented in Table 2. In the same study, it was shown that the micro-indentation response was different within an interphase of 1 µm. Also, based on systematic experimental and computational analyses of DP600, Ramazani et al. [71] showed that the thickness of this interphase where GNDs are stored is on the order of 1 µm. Hence, it will be assumed first that the interphase thickness is 1 µm for the simulated RVEs.

Three virtual RVEs are generated with different martensite island sizes, but with approximately the same $V_{f,M}$ of 40% as shown in Fig. 23. All the RVEs consist of an interphase region of 1 µm thickness with the exception of Fig. 23(d) in which the interphase is 2 µm thick which is assumed in order to study the effect of the interphase thickness on the overall response while the martensite phase size is set constant. Table 3 shows the volume fraction of each phase for the three virtually generated RVEs (Fig. 23(a) and (c)).

In our first study, three cases are considered for the virtual RVE of the largest martensite island size (7 µm): (1) the material properties of the interphase are assumed to be the same as the ones of the ferrite phase, i.e. no interphase, (2) the interphase material
properties (see Fig. 22) are imposed for the interphase region, and (3) the material properties of martensite are assumed for the interphase region, i.e. no interphase but higher $V_{f,M}$.

Fig. 24(a) clearly shows that there is a noticeable change in the mechanical behavior for all three cases. The highest strength and lowest ductility are obtained when the interphase region is modeled with the martensite property; which is expected. The comparison between the interphase being modeled as a ferrite verses...
being modeled with its measured properties reveals how the results can differ if the assumption of constant ferrite properties is taken into account. Including the interphase with different properties clearly yields the size effect of the martensite phase while keeping its volume fraction nearly constant. Also, it shows higher UTS but lower ductility.

In the second study, the effect of interphase thickness is investigated for the RVE with the largest martensite island size of 7 μm. Three cases are considered: (1) 1 μm thickness, (2) 2 μm thickness, and (3) the mechanical properties of the ferrite phase are taken as the properties of the interphase region, i.e. no ferrite phase, or the whole interphase is occupying the ferrite phase which is expected when the martensite phase is very fine, or equivalently the thickness of the interphase is very large.

Table 3
Comparing volume fraction of various martensite island sizes with interphase region in the ferrite matrix.

<table>
<thead>
<tr>
<th>Martensite island sizes (μm)</th>
<th>Ferrite</th>
<th>Interphase</th>
<th>Martensite</th>
</tr>
</thead>
<tbody>
<tr>
<td>7</td>
<td>21.88</td>
<td>31.55</td>
<td>38.55</td>
</tr>
<tr>
<td>5</td>
<td>8.89</td>
<td>53.00</td>
<td>38.10</td>
</tr>
<tr>
<td>3</td>
<td>2.53</td>
<td>57.51</td>
<td>39.94</td>
</tr>
</tbody>
</table>

Fig. 23. Virtual RVE with 1 μm interphase between ferrite and martensite for varying martensite phase sizes of (a) 3 μm, (b) 5 μm, and (c) 7 μm and (d) 2 μm interphase of 7 μm martensite phase size while keeping the $V_{IM}$ constant at 40%.

Fig. 24. Macroscopic response of RVE of 7 μm martensite phase size with (a) varying interphase properties and (b) increasing the interphase size.
The effect of interphase thickness is illustrated in Fig. 24(b). When the interphase thickness is increased the results show that the strength and the ductility increase simultaneously, which is a very interesting result. This is attributed to that the interphase material property exhibits a higher hardening rate along with a higher strength as compared to the ferrite phase.

In the third study, the martensite phase size is decreased while keeping a constant 1 \( \mu \)m thickness for the interphase. The measured interphase material properties by Ghassemi-Armaki et al. [37] are assigned to the interphase. The RVEs for this study are shown in Fig. 23(a)–(c) while the results are shown in Fig. 25. It is seen that as the martensite phase size decreases, the overall behavior of the DP steel becomes stronger and more ductile. This is because the volume fraction of the ferrite–martensite interphase increases with the decrease of martensite phase size (see Table 1). These simulation results agree well with the experimental observations by Erdogan and Tekeli [29] that showed that both the tensile strength and the ductility increased with decreasing the martensite phase size at constant martensite volume fraction.

Fig. 26 shows the equivalent plastic strain of the third study above. Multiple shear bands are visible in all the three virtual RVEs; however, the shear bands for the largest martensite islands are more intense and thicker. Furthermore, the evolution of the voids can be noticed clearly for the 5 \( \mu \)m and 7 \( \mu \)m martensite phase sizes along the shear bands. As for the 3 \( \mu \)m martensite phase size, the shear bands are more distributed which contribute to increased strength and ductility.

It is noteworthy that, based on a combination of experimental and computational analysis, Ramazani et al. [71] have suggested three criteria for modeling the interphase at the ferrite–martensite boundary in which GNDs are initially stored during the fabrication process of DP steels. The first criterion suggests that the strength of the interphase is almost 1.3 times the strength of the ferrite. This criterion is already included in the first parametric study as the experimental data from micro-pillars compression (see Fig. 22) shows that this ratio is around 1.4. The second criterion suggests that the thickness of the interphase is almost 25% of the martensite
particle size. This criterion is also taken into consideration in the second and third parametric study of this section where the case of increasing the interphase thickness while increasing the martensite phase size is considered. See the results in Figs. 24 and 25 where for 5 μm martensite particle size 1 μm interphase thickness is assumed whereas for 7 μm martensite particle size 2 μm interphase thickness is assumed. In fact, the results from this criterion are almost the same. Finally, the third criterion states that the equivalent plastic strain in the interphase is 1.3 times that in the ferrite grain. Although this criterion is not tested in this paper, we believe that it is equivalent to the first one and will yield similar results.

3.7. Effect of ferrite grain size

In this section, the effect of ferrite grain size on the overall response of DP steel will be discussed. The grain size effect of the martensite phase is not investigated here since the mechanical behavior of the martensite is much stronger than the ferrite such that this effect is not expected to significantly influence the overall behavior of the DP steel.

Three virtual RVEs are generated of 40% \( V_{f,M} \) with varying grain sizes of 7 μm, 5 μm, and 2 μm. The RVEs are presented in Fig. 27. The methodology used for modeling grain boundaries is the same used in the previous subsection for modeling the martensite–ferrite boundary which is the "core and mantle" method. This is done through creating a finite thickness interphase at the grain boundaries. For this study, it is assumed that no yielding takes place at the grain boundaries (i.e., hard boundary) by assigning a very high yield strength to this region. This is the commonly adapted assumption in modeling grain–grain boundaries (e.g., [10,13,30,88]). An intermediate (i.e., not hard and not free) grain–grain boundary behavior, which is more realistic, can be assumed as well (e.g., [2,33]). Moreover, grain boundary sliding/debonding is not considered here. However, due to the lack of experimental data that characterizes the mechanical behavior of the ferrite grain–grain boundary in DP steels, which is needed to calibrate such grain boundary conditions, the hard boundary assumption is adapted here. Data from atomistic calculations (e.g., [81,85]) might be useful in calibrating more realistic continuum-based modeling of grain boundaries.

Fig. 28 compares the stress–strain responses for DP steels with varying grain sizes. As commonly observed (e.g., [17,50,62]), the simulation results reveal that the strength of DP steels increases when the grain size decreases; however, it is coming on the expense of ductility. Fig. 29 indicates the tensile strength and the ductility are functions of the grain size. The corresponding strain at UTS as a function of grain size does not follow a clear trend rather it seems to be constant.

Fig. 30 represents the equivalent plastic strain for all the three RVEs with different grain sizes. It is clear that shear bands are disconnected due the grain boundaries. Moreover, the shear bands for grain size 7 μm and 5 μm are thicker and more localized as compared to those for 3 μm. However, cracking seems to occur more for the 3 μm grain size explaining the decrease in ductility.

4. Conclusions

In this paper, a microstructure-based finite element modeling approach is adopted to examine the key factors of microstructure
that influences the overall behavior of DP steels. A unique approach in mimicking the microstructure was investigated and validated with real SEM based RVEs. The results showed that the virtual RVE can predict the mechanical behavior effectively.

The issue of mesh sensitivity, which is generally not addressed by the studies on microstructural modeling of DP steels, is greatly reduced through using the viscosity-regularization. This method does not increase any computational cost and is simple and very easy to adapt. It is noticed that through using the viscosity-regularization approach, the DP ductility increased significantly without compromising its strength. Through adding small amount of viscosity or by making the material time-dependent, the ductility increased by more than 50%.

The effect of the martensite–ferrite interphase properties and thickness on the overall mechanical behavior of DP steels were investigated. It was shown that the strength and ductility change significantly when the interphase properties and thickness are altered. It was also shown that the size of the martensite does affect the overall behavior when taking the interphase into account. This size effect shows that both strength and ductility of the DP steel increased with decreasing the martensite phase size at constant martensite volume fraction and constant interphase thickness. This type of size effect is desirable as it leads to simultaneous increase in strength and ductility of DP steels.

By assuming hard ferrite grain boundaries, it was shown how the grain size affects the overall mechanical behavior of DP steels. It was seen that the strength increases significantly when the grain size is decreased; however, with the compromise of ductility. The methodology that was adapted in modeling the grain boundaries, “core and mantle” approach, conveniently reflects the effect of the grains in DP steels in a simple manner.

This paper dealt with other minor parametric studies as well. The effect of martensite distribution was studied, which showed that the distribution has no effect on the overall mechanical response of DP steels. The effect of volume fraction of martensite was also studied, which showed that as the volume fraction of martensite increases the strength increases while the ductility decreases. The effect of martensite size without the interphase was also studied, which showed that a higher-order plasticity theory needs to be implemented to capture this size effect.

Lastly, it is noticed in this paper that the failure mode was due to plastic strain localization in the form of localized narrow bands. Micro-voids were formed in these localized zone which significantly controlled the overall ductility.

References