Multiscale Model Analysis of the Effects of Martensite Morphology and Martensite Volume Fraction on the Mechanical Property of Dual-Phase (DP) Steels: Parametric Study

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Abstract

Multiscale material modeling is important for directing the material design of heterogeneous materials with concurrent improvements in mechanical properties. In this study, the plastic deformation of DP steels with different microstructures features namely martensite aspect ratio, and martensite volume fraction was investigated. A new methodology that studies the effects and interactions of martensite aspect ratio (equiaxed versus elongated) and martensite volume fraction on the mechanical behavior of DP steels was developed. A multiscale material and structure model using a dislocation density based nonlinear elastic-viscoplastic model was used to predict the mechanical behavior of DP steels under quasi-static loading condition. A comprehensive parametric study using response surface methodology (RSM) model were conducted on the influences and interactions of the considered microstructure parameters in DP steels on the energy absorption capacity. This methodology utilizes a microstructure-based approach using a multiscale material and structure model, in which Digimat and LS-DYNA® software were coupled and employed to provide a full micro-macro multiscale material model to perform simulated tensile tests. The numerical results are validated using experimental data found in the literature. The developed methodology proved to be effective for investigating the influence and interaction of key microscopic properties on the mechanical properties of DP Steels and thus can be used to identify optimum microstructural conditions

Introduction

The development of a clear understanding of the influence of various microstructural parameters on the overall behavior of DP steels is required to enhance the crash resistance and reduce body car weight and meet the increase in use of dual phase (DP) steels grades by car manufacturers [1–3] . The microstructure of DP steels consists of martensite phase particles dispersed in the soft ferritic matrix. Several works have been published that investigates the effect of microstructural parameters on the overall behavior of DP steels (e.g., [1–9]). Nevertheless, notwithstanding the concentrated research efforts, there remains one important key microstructural parameter that has not been studied comprehensive, computationally, in spite of its significant effect morphology of the martensitic phase [10]. However, although these research and others have extensively investigated the effect of microstructure parameters on the overall of DP steels both computationally and experimentally, there is a need for a comprehensive statistical study of the effect of the martensite morphology and volume fraction and the role they play in affecting the mechanical property of DP steels.
To the author's best knowledge, no detailed comprehensive statistical study has investigated the morphological parameters on strength and ductility of DP steels namely martensite elongation (i.e., aspect ratio (AR)) and different directions of rolling (Dir) (i.e., rolling direction (RD) & transverse direction (TD)). These are some of the few parameters along with other microstructural parameters (i.e., martensite volume fraction (V_m)) that will be discussed in this paper.
To that end, a multiscale material modeling approach of DP steels is utilized along with a statistical and mathematical tool to create an efficient analytical methodology for studying the influence of the morphological parameters and martensite volume fraction under quasi-static loading conditions, which is presented in the author's previous work [1–3].

Multiscale Material & Structure Modeling

Digimat-CAE (i.e. the linear and nonlinear multiscale material modeling software from e-Xstream engineering) that facilitates the coupling between the mean-field homogenization incremental formulation Digimat-MF and LS-DYNA is employed to simulate the flow behavior of DP steels in uniaxial tension under quasi-static loading. The model is then used to conduct a parametric study using response surface methodology (RSM) on the influence of AR, Dir and V_m on the mechanical property of DP steels under quasi-static conditions. Specifically, a dislocation density based nonlinear elastic-viscoplastic model that can predict the flow stress of DP steels under quasi-static uniaxial loading conditions is developed. After performing the simulation, the parametric study was conducted on the influence of AR, Dir, and V_m on the inelastic behavior. This is followed by a systematic response surface methodology (RSM) investigation of the effect of AR, Dir and V_m on the flow stress of DP steels as well as an evaluation of the effective microscopic factors. In addition, the optimum values of microstructure parameters are derived for achieving the maximum strength as well as highest ductility. A mean-field homogenization incremental formulation (Digimat-MF) that targets to predict the flow stress of DP steels based on the constitutive equation of ferrite and martensite phase is used to link LS-DYNA through LS-DYNA user-defined material (UMAT) code as shown in Fig. 1. LS-DYNA is executed at the macro-scale, and for each time interval at each integration point (IP) of the macro FE mesh, LS-DYNA/UMAT calls Digimat-MF through Digimat-CAE to carry out the homogenization technique of two phases (ferrite and martensite) as shown in Fig. 1. Detailed constitutive equations that were used in this paper were presented in the author's previous work [2,3] where the dislocation density constitutive formulation as the typical relationship of the flow stress based on dislocation density was used to describe ferrite and martensite flow stress. A Mori-Tanaka model was used as homogenization technique, which supposes that the inclusions in the RVE undergo the matrix strain as the far-field strain in the Eshelby's solution [1–3,11].

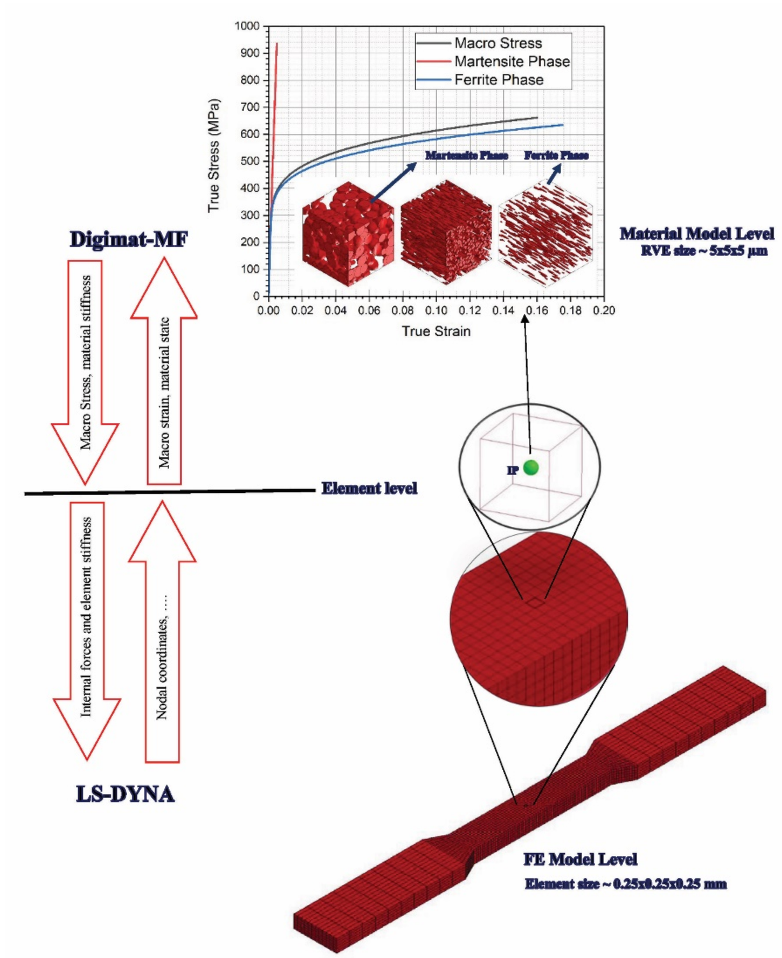


Fig. 1: Multiscale material modeling using Digimat as the material modeler and LS-DYNA as structural FEA software

Response Surface Methodology (RSM)

RSM is used as a statistical design of experiments, which refers to the methodology of arranging the tests so that the appropriate data can be examined comprehensively and statistically [1–3]. RSM was used in this study to investigate the relationship between a response variable and a set of factors. The required analysis points (the simulation settings) within specified ranges of the morphological parameters and martensite volume fraction were defined by using RSM: an AR range of 1 – 7, a Dir range of RD and TD, and a V_m range of 3.3 – 47%. The ranges of these factors (AR, Dir and V_m) were estimated based on the previous literature review [1–3,12,13] and few preliminary trials. Detailed RSM model that was used in this paper were presented in the author's previous work [2,3] where the analysis design matrix based on the Central Composite approach was generated using MINITAB software after the design factors, and their ranges had been introduced. Consequently, the multi-scale material modeling was conducted according to the analysis design matrix listed in Table 1 which was obtained by the RSM model, and a tensile toughness was then introduced into the previously designed matrix as a response in that analysis.

Table 1: Design of analysis matrix using MINITAB software

Design Points	Factors		
	Dir	**AR**	**V_m**
DP#1	RD	1	25.15
DP#2	TD	1	25.15
DP#3	RD	7	25.15
DP#4	RD	7	3.30
DP#5	TD	7	25.15
DP#6	TD	4	25.15
DP#7	RD	4	3.30
DP#8	TD	4	3.30
DP#9	RD	7	47.00
DP#10	TD	4	25.15
DP#11	RD	4	25.15
DP#12	RD	4	25.15
DP#13	TD	7	47.00
DP#14	TD	7	3.30
DP#15	TD	1	3.30
DP#16	TD	4	47.00
DP#17	TD	4	25.15
DP#18	TD	1	47.00
DP#19	RD	4	25.15
DP#20	RD	1	47.00
DP#21	TD	4	25.15
DP#22	RD	4	25.15
DP#23	RD	4	25.15
DP#24	RD	1	3.30
DP#25	RD	4	47.00
DP#26	TD	4	25.15

Methodology

In this paper, the micro-macro multiscale material modeling was conducted to obtain the flow stress of DP steels, which are considered composite materials consisting of martensite islands as inclusions and a ferrite phase as a matrix as mentioned earlier. The whole simulation procedure was performed using MINITAB (RSM), OriginLab (Data management tool), Digimat software (Mean field homogenization), and LS-DYNA (FE software). Coupling Digimat-MF to LS-DYNA via UMAT/Digimat-CAE was performed and loading and boundary conditions were defined in LS-DYNA. The flow curve of the micro-macro multiscale material model for each design point in Table 1 was obtained using coupling Digimat-MF to LS-DYNA. An analysis of the RSM model by adding tensile toughness for each design point to the design of the analysis matrix was carried out to obtain the comprehensive statistical parametric study, and the microstructure parameters optimization. itemized implementation steps of this methodology that were used in this paper were listed in the author's previous work [2,3]. The micro-structure of two phases are not "seen" by LS-DYNA but only by Digimat-MF, which takes into account each integration point (IP) to be the center of a representative volume element (RVE) which contains the heterogeneous micro-structure of two phases as shown in Fig. 1. Digimat-MF generated RVEs where the martensite islands were designed as inclusions and ferrite phase as the matrix in DP steels and were simulated as the ellipsoid model, and aspect ratio (AR), rolling direction (RD or TD), and volume fraction (V_m) of the martensite islands were both defined through the Digimat model as shown in Fig. 2.

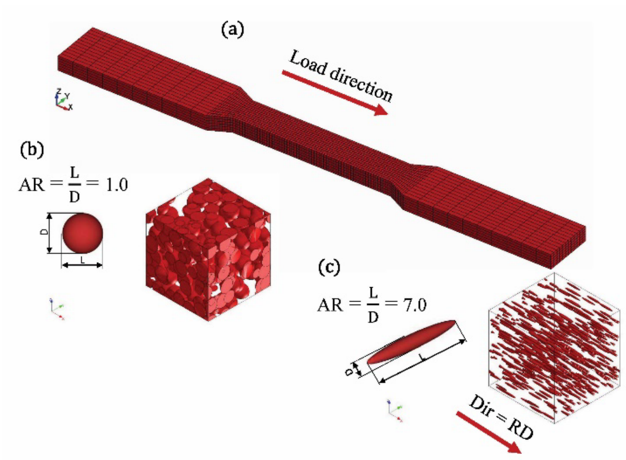


Fig. 2: (a) A standard ASTM E8 specimen geometry with load direction (b) RVE with AR=1, Dir=RD, and V_m=47% (DP#20), and (c) RVE with AR=7, Dir=RD, and V_m=3.3% (DP#4)

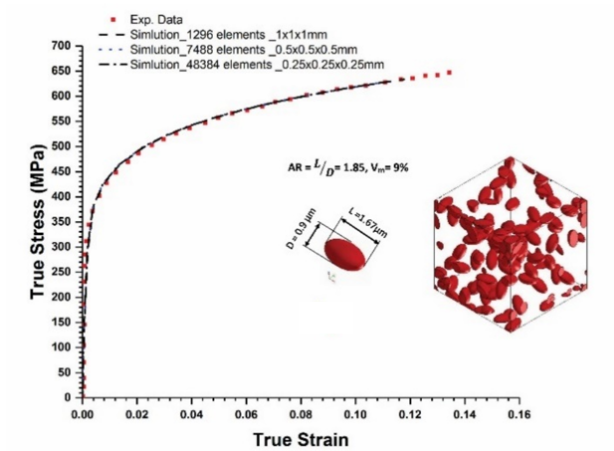


Fig. 3: Comparison between the experimental and numerical results at specific microstructure parameters (AR= 1.85, Dir= random 3D, and V_m= 9%) [14] and different mesh size

Results and Discussion

Each simulation point (design point) was conducted according to conditions in the design matrix in Table 1. The experimental data that contained statistical quantitative metallography and the stress-strain curve of DP500 at a 0.14 sec^{-1} [14] were compared to the predicted numerical stress-strain curves at different mesh size to estimate the accuracy of the simulation results as shown in Fig. 3. As can be seen in Fig. 3, the simulation results are mesh independent and in good agreement with experimental results.

Stress–strain curves for all the 26 design points in the design matrix (Table 1) are presented in Fig. 4. It is obvious that the Stress–strain curves are different due to changing the morphological parameters and martensite volume fraction. A complete quadratic model was chosen to investigate RSM using MINITAB software after adding tensile toughness as the responses in the designed analysis matrix as shown in Table 1. The analysis of variance in Table 2 that summarizes the statistical significance of each factor was presented briefly in Tables 2. The small p-values for aspect ratio (AR), martensite volume fraction (V_m), and direction of rolling (Dir) indicate that these effects are statistically significant on tensile toughness. On the other hand, the small p-values for the square terms of $(AR)^2$ and $(V_m)^2$ indicate that these effects are a certain trend toward quasi-significant because these factors have large p-values. In Table 2, The R^2 and adjusted R^2 show that the model fits the data well. The Interaction graph that generates a matrix of interaction graphs for the considered factors for tensile toughness is shown in Fig. 5.

Term	P-Value
Constant	0.000
AR	0.000
Dir	0.000
V_m	0.000
AR * AR	0.476
V_m * V_m	0.816
AR * V_m	0.002
AR * Dir	0.000
V_m * Dir	0.000
Linear	0.000
Square	0.769
2-Way Interaction	0.000
Lack-of-Fit	0.130
R-sq	**R-sq (adj)**
93.00%	91.01%

Table 2: Analysis of Variance (ANOVA) results of the statistical significance of each

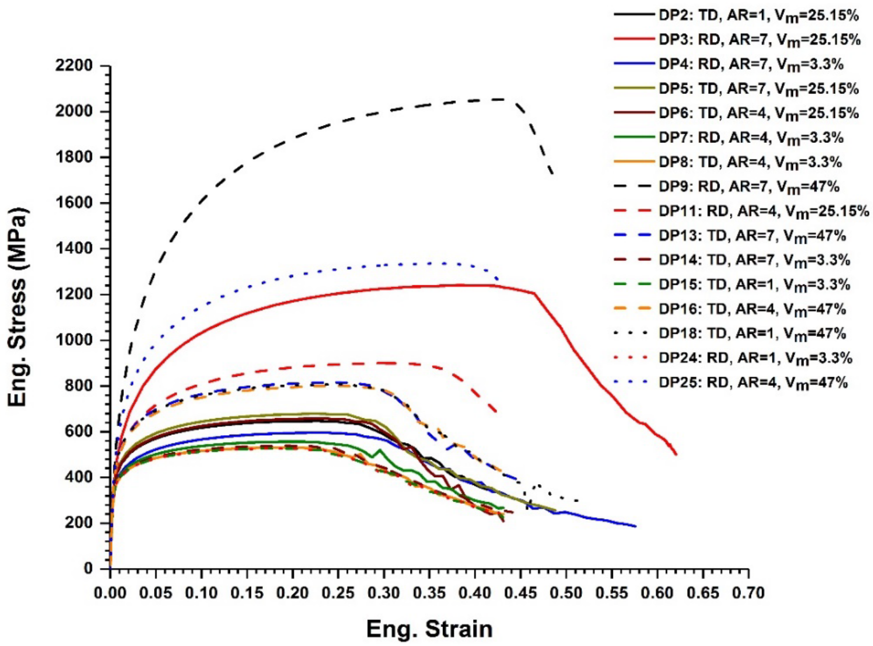


Fig. 4: Numerical stress–strain curves for all design points in the analysis

It can be seen that the interaction graphs are a graph of each response mean for each level of the considered factor with the other factors kept constant, which is helpful for estimating the presence of interaction among the considered factors. As follows from the interaction graphs shown in Fig 5 the parallel lines in an interaction graph signify no interaction; however, the interaction exists in case the lines are not parallel.

The greater the difference in slope between the lines, the higher the level of interaction. The parametric study conducted by the RSM model, and the effects of the considered factors on the response are shown in Fig 6 to Fig 7 as 2D contours and 3D surface plots that were generated by MINITAB software. All these plots are kept and identified at the middle level of factors, which shows how the fitted response relate to two considered factors. The provided graph in Fig 6 (a) shows the tensile toughness increases gradually with rising V_m; while the tensile toughness moderately increases with decreasing AR. The 2D contour, Fig 6 (b), shows that increases in toughness from the lower range to the higher range of V_m, on the other hand, increases in toughness from the higher range to the lower range of AR.

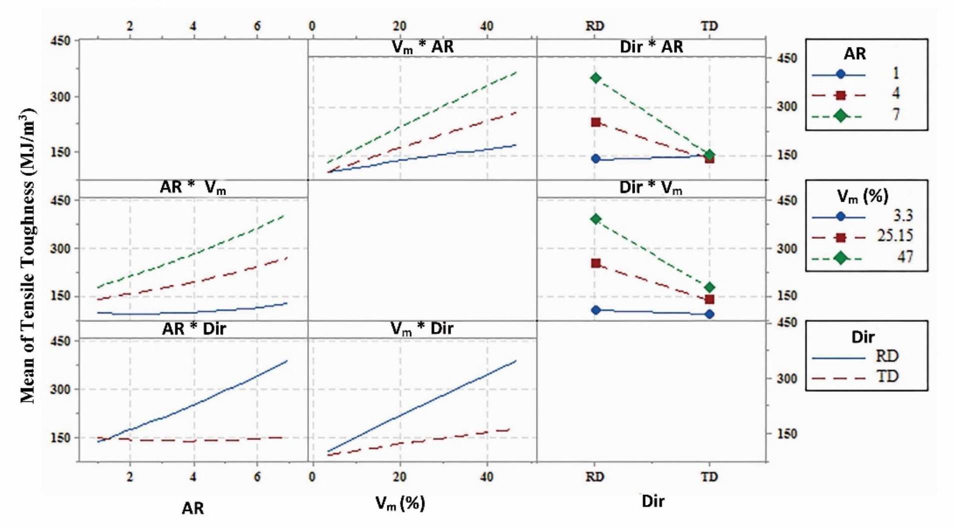


Fig. 5: Interaction Plots for tensile toughness (fitted means)

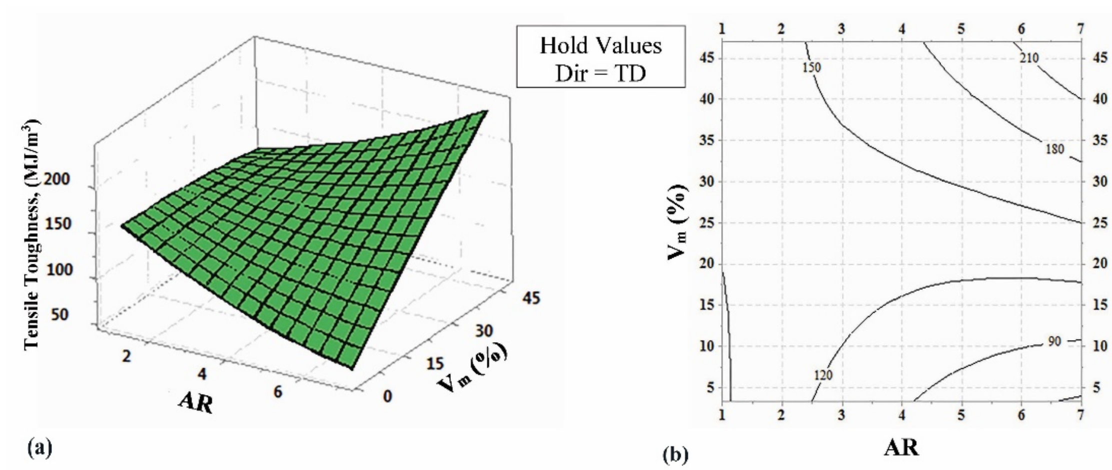
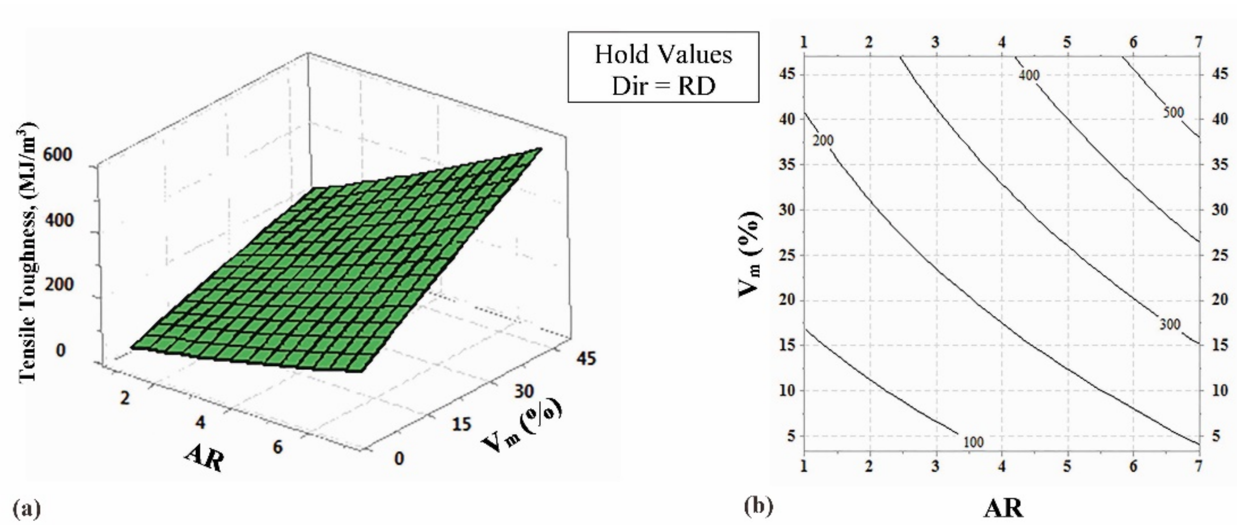


Fig. 6: (a) 3D surface plot of response surface showing the effect of aspect ratio (AR), martensite volume fraction (V_m), and their mutual effect on toughness at Dir = TD; (b) corresponding 2D contour plot.

The 3D surface plot in Fig. 7 (a) demonstrates that the rise in toughness from the low to the high level of V_m is larger at the higher values of AR. Another key point to remember in Fig. 7 (b) is that the 2D contour plot indicates that the largest toughness is achieved when AR and V_m values are high. This highest toughness range shows at the upper right corner of the plot, which is greater than 500 MJ/m^3.



(a) (b)

Fig. 7: (a) 3D surface plot of response surface showing the effect of aspect ratio (AR), martensite volume fraction (V_m), and their mutual effect on toughness at Dir = RD; (b) corresponding 2D contour plot.

In order to sum up the results in Fig 6 and 7, the increase in V_m can significantly affect the response – toughness – where the toughness increases significantly with rising V_m at higher values of AR in both rolling direction RD and TD. On the other hand, it may be clearly seen that for the toughness of DP steel at the lower values of V_m and rolling direction (TD), the lower values of AR have a higher effect on the toughness more than the higher values of AR, and vice versa.
To put it another way, through the study that used, for the first time, comprehensive statistical parametric study, we found that the effect of aspect ratio (AR) has different influence on the energy absorption capacity of DP steels based on the martensite volume fraction (V_m). Moreover, the martensite volume fraction (V_m) is clearly a more considerable influence than the effect of aspect ratio (AR).

Conclusions

In this paper, the full micro-macro multiscale material modeling based on mean-field homogenization incremental formulation and the response surface methodology (RSM) was used to investigate the effects of the morphological parameters and martensite volume fraction using an elasto-viscoplastic constitutive model for each phase in the DP steel. Not only numerical prediction from the full micro-macro multiscale material modeling was in good agreement with the flow curve of DP500, but also the model contributes further understanding into improving the energy absorption capacity of DP steels under quasi-static. The parametric study based on the effect of variations of the morphological parameters and martensite volume fraction revealed that these factors play an important role in the mechanical behavior of DP steels. It was shown that for these factors, the energy absorption capacity of material would be optimized.

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