MULTISCALE MODELING AND SIMULATION OF THE MECHANICAL BEHAVIOR OF THE DUAL PHASE STEELS: PARAMETRIC STUDY AND MICROSTRUCTURE OPTIMIZATION

By

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To the Faculty of Washington State University:

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The goal of this thesis is to investigate the relationship between microstructure properties and mechanical properties of dual phase (DP) steels to design advanced materials for automotive applications. In this research, a new effective analytical methodology that studies the influences and interactions of microstructure properties on the mechanical behavior of DP steels under different strain rates was developed. In this work, the plastic deformation of multiphase material with different microstructures including volume fraction and grain size of phases, and carbon content in DP steels etc., under different strain rates was investigated.

First, a microstructure-based approach using a 3D micromechanical model was suggested. The 3D representative volume elements (RVEs) model that can precisely predict the mechanical behavior of DP steels under quasi-static strain rate is developed. This is followed by a methodical response surface method (RSM) to investigate the effects and interactions of microstructure parameters on the mechanical behavior of DP steels. The developed method can estimate effective microscopic parameters, as well as optimum values of microstructure features for achieving the maximum energy absorption capacity of DP steels. Through the comprehensive parametric study,
it was shown that the microscopic parameters play an important role in the mechanical properties of DP steels, as well as the energy absorption capacity of material would be optimized.

Second, a multiscale material and structure model using a dislocation density based nonlinear elastic-viscoplastic model was developed to predict the mechanical behavior of DP steels under quasi-static and dynamic uniaxial loading conditions. A comprehensive parametric study and microstructure optimization using RSM model were conducted on the influences and interactions of microstructure parameters in DP steels on the strength, ductility, and energy absorption capacity. It is shown that the microscopic parameters and their two-way interactions play an important role in the mechanical behavior of DP steels, as well as the strength, ductility and tensile toughness of DP steels, would be optimized. Furthermore, not only did this methodology is a powerful tool to investigate the microstructure parameters effects at various strain rate conditions and an effective optimizer tool, but it is also possible forming operations and collision-related data.
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Dedication

This dissertation is proudly dedicated

To my mother, Selima Saleh,

To memory of my father, Mahmoud Belgasam,

To my wife, Samia Fadil,

who provide endless support and love during my life and Ph.D study

To memory of two close friends,

Mohammed Hussein and Mohammed Jomaa,

who were my siblings I chose for my life

To memory of my MSc. advisor, Dr. Ata Al-khatib,

who left a fingerprint in my academic life
CHAPTER ONE: GENERAL INTRODUCTION

1.1 Automotive materials

The growth automobile marketplace demands for cut down fuel consumption as well as reducing greenhouse gas emissions (GHG) and use of raw resource and increasing recyclability have forced the automobile industry to adopt more effective method of fuel consumption by decreasing body car. To increase safety, strength and reduce fuel consumption along with an increase in the crashworthiness performance require extraordinary materials with suitable combinations of strength, ductility, and durability. To put forward these requirements, steelmakers seek new steels to improve ductility and maintain increases in strength. In order to comply with the international environmental regulations, a new car architecture based on using thinner gauges of sheet material have been developed. In an effort to comply with the demands of automotive manufacturers, steelmakers have used advanced high strength sheet steels (AHSS) with a better strength-ductility combination and low cost. The application of AHSS have exhibited an exceptional preference of combining vehicle weight reduction (by using thinner gauges of sheet AHSS), with improved crashworthiness performance and good formability at reasonably priced cost [3–5]. AHSS are most beneficial when used for better safety, fuel efficiency, environmentalism, formability, ductility, and features. Generally, using AHSS reduces weight by about 50% compared to mild steel; the width is halved without losing strength [3].

AHSS are multiphase material that contains hard particles of martensite, bainite phase and/or austenite phase spread in a ductile ferritic matrix, in amounts and mixtures adequate to produce desired mechanical properties. Many different grades of AHSS have been developed, and the descriptive terminology of AHSS has been developed to explain the first generation of AHSS, ferritic microstructure-based, and the second generation of AHSS, i.e., austenitic microstructure-
based that contain high manganese, which includes steels that are related to austenitic stainless steels. First generation AHSS are comprised of transformation-induced plasticity (TRIP), dual phase (DP), complex phase (CP), and martensitic (MART) steels. Whereas the most important grade of the second generation austenitic AHSS is twinning induced plasticity (TWIP) steels [3,6].

Due to their unique microstructure properties, DP steels with ferritic-martensitic microstructure make available a desirable strength/ductility combination and continuous yielding behavior accompanied with a high work hardening rate. The simplest method to produce DP steels with ferritic-martensitic microstructure is an intercritical heat treatment of a ferritic-pearlitic microstructure in the α + γ two-phase region. DP steels mechanical properties variation comes from different microstructure features and alloying elements, which can be controlled by carbon content in steel, appropriate annealing scheduling, and adding alloying elements. For these reasons, various DP steels grades are produced industrially to meet distinctive design requirements of vehicle components. The high marketable possibility of DP steels has motivated myriad studies in numerous research laboratory, resulting in a wide range of DP steel grades with different chemical compositions and being produced with several processing ways [7–12]. Three basic commercial methods exist for producing DP steels, which includes [13–16] :

1) Conventional hot-rolling cycle method
2) Hot or cold rolled steel strip method
3) The batch annealing method

Continuous yielding behavior, low yield stress, high tensile strength, high uniform tensile ductility and high work hardening are important mechanical properties of DP steels. These superior mechanical properties come from microscopic characteristics, which is the fine spreading of hard islands of martensite phase in the ductile matrix of ferrite phase and all the related aspects
that accompany with this phenomenon. The high dislocation densities and residual stress occurring in ferrite phase have contributed in the continues yielding and high work hardening due to the volume expansions accompanying with austenite to martensite transformation. The volume fraction and carbon content of martensite phase are primarily responsible for the strength of DP steels, as well as alloying elements. The ductility for most DP grades was found to be depended primarily upon many factors, which is among them are the volume fraction and carbon content of martensite phase, and the alloying elements in ferrite phase [17–27].

As mentioned previously, DP steels are well known for their high strength and ductility balance; as a consequence, they are extensively used in the automobile industry. Recently, there has been a growing need to find a third generation of AHSS that are characterized by strength and formability balance more than that presented by the first generation of AHSS, but at a lower cost than that needed for the second generation. In the past, different routines have been tried to expand the wide range between the first and second generations of AHSS. Within those methods, multi-phase material modeling (computational methods) [8,28–32] and quenching & partitioning (Q&P) methods (experimental methods) [4,33–35] have been dominant. These methods are used to develop new DP steels through predicting and optimizing microstructure features to design the unique mechanical properties features of the third generation of AHSS. Thus, the third generation is one area of particular current interest to reduce the disparity of strength-ductility combination between the first and second generation [36]. In order to develop DP steels and predict the third generation of AHSS, a review of the previous work is essential. The mechanical properties of DP steels could be controlled by changing volume fraction of phases [8,28–30,32,33], as well as size and morphology of phase elements [28,32–34]. Although these previous research have extensively studied DP steels both computationally and experimentally, there is still a need for an inclusive
statistical investigation of the influence of basic microscopic characteristics and the role they play in affecting mechanical properties and the strain rate sensitivity of DP steels.

To that end, an effective methodology for investigating the influences and interaction of microstructure properties of DP steels on the mechanical behavior of DP steels was developed and therefore can be used to obtain optimum microstructure parameters at different strain rate conditions. A micro-macro multiscale material model based on mean-field homogenization (Digimat-MF) coupling with a general-purpose finite element program (LS-DYNA) was developed to predict the flow stress of DP steels. The simulation results are then used to carry out a comprehensive statistical parametric investigation by using response surface methodology (RSM) on the impact and interaction of various microstructure parameters on plastic behavior of DP steels under different strain rate conditions and then to determine the optimum microstructure parameters for a required combination of strength/ductility.

1.2 Multiscale material model

In general, a multiscale material model is the field of solving problems, which has important microstructure characteristics at multiscale of time and/or space. The challenged analysis when conducting FE analyses with the multiphase materials is to predict the mechanical behavior of DP steels based on the interaction between the microstructure parameters and the macroscopic properties. Thus, it is appropriate to separate between two scales; the microscopic scale, where the multiphase material it treated as heterogeneous material, and the macroscopic scale, where the multiphase material is treated as locally homogeneous material, which can be predicted based on micromechanical modelling. Many technologies can be used to predict multiphase material behavior across scales, all with their own advantages and disadvantages [37,38]. The multiscale
material model allows to simulate multiphase material, DP steels, using more accurate microscopic constitutive laws.

In this research, the so-called mean-field homogenization (MFH) technique, Mori-Tanaka (MT) scheme, that uses Eshelby’s solution to predict the macro-field was used, which is supported in Digimat-MF and because it is very CPU cost-effective [39]. The “Digimat” software (i.e., The Linear and nonlinear multiscale material modeling software from e-Xstream engineering) and its interface to structural FEA software facilitate multiscale finite element analysis of DP steel microstructure under different strain rates. The Digimat-CAE that sets the interface between the mean-field homogenization incremental formulation (Digimat-MF) and structural analysis software (LS-DYNA) is used to accurately predict the flow behavior of DP steels in uniaxial tension under quasi-static and dynamic loading. Digimat-MF as a software library that is linked to LS-DYNA via LS-DYNA’s user-defined material to offer a full multiscale material coupling between the nonlinear micromechanical material modeling abilities of Digimat-MF and the nonlinear structure FE capabilities of LS-DYNA as shown in Figure 1.1.

Figure 1.1: Multiscale material model: general workflow
In this design, Digimat-MF implements as an advanced multiphase material model, nonlinear and rate-dependent user-defined material at each integration point of the LS-DYNA FE mesh. To generate an accurate material model in Digimat-MF, some required material constants should be known, and others should be determined. The material constants that should to be known in this case are both the density of the matrix, ferrite phase, as well as material constants for the isotropic and elastic inclusions, martensite phase, i.e., modulus of elasticity, density, Poisson’s ratio and the aspect ratio (AR) of martensite particles. The material constants that have to be determined by reverse engineering (RE) in this case are material constants for the ferrite phase as matrix required to fit the material model, e.g., modulus of elasticity, yield stress, Poisson’s ratio, hardening constants and viscoplasticity constants. The output from the multiscale material model is an adjusted material model to be implemented in the structure FE model by LS-DYNA [40].

In Digimat-MF, the linking between the microscale and macroscale depends on the rule of so-called representative volume elements (RVE). Each RVE represents to a single material point on the macroscopic scale, which should be large enough to represent the heterogenic multiphase material but small enough related to the homogeneous material. The Digimat-MF approach that allows for a connection between the two scales is presented in Reference [41].

1.3 Response surface methodology (RSM)

The comprehensive statistical parametric study and optimization is the key step to investigate the effects of a set of variables on the responses and to obtain optima of the desired responses in any experimental field. Traditionally, a simplest classical parametric study (one at a time) that investigates changing one independent variable while maintaining all others at a fixed level is extremely laborious for many variables and takes too much time, as well as the lack of presence of the interactive influences among variables. Recently, RSM has been extensively
utilized as a comprehensive statistical tool for parametric study and optimization in various kinds of analytical science fields and industrial processes [42].

The RSM is a group of statistical and mathematical approach advantageous for analyzing and investigating of problems in which a response is affected by many variables, and the purpose is to maximize/minimize this response [43]. Not only did the RSM is the statistical design of experiments, but it is also used for investigating, developing, and optimizing the response variable. For example, the energy absorption capacity of DP steels is affected by microstructure parameters \((x_1, x_2, x_3)\) and strain rate \((x_4)\). In this case, the energy absorption capacity of DP steels \((y)\) is the response variable, and it is a function of the microstructure parameters and strain rate as follows:

\[
y = f(x_1, x_2, x_3, x_4) + e
\]  

(1.1)

where the variables \(x_1, x_2, x_3, x_4\) are independent variables and \(e\) is the experimental error, which the response \(y\) relies on them. This experimental error represents any estimates error on the response, as well as other type of variation not counted in the function \(f\), which is a statistical error that is supposed to distribute data normally with zero average and variance. In most RMS models, the response function \(f\) is unknown and in order to estimate an appropriate approximation for it, the RSM examines the data first if a low order polynomial model fits data well. If there is a curved surface in the response surface, complete order polynomial equation is advantageous in estimating a portion of the true response surface with curvature. The complete order polynomial model contains all the terms in the low order polynomial model, and quadratic and cross product terms, which can be expressed as [42–44]:
\[ y = \beta_0 + \sum_{i=1}^{n} \beta_i x_i + \sum_{i=1}^{n} \beta_{ii} x_i^2 + \sum_{i>j} \beta_{ij} x_{ij} + e \]  

To get the most effective results in the RSM model, the appropriate experimental or computational data should be employed to generate analysis design data. Once the analysis design data are generated, the Least Square method is utilized to estimate the coefficients in the polynomial model, and then the response surface analysis is conducted by means of the fitted surface. Therefore, the objective of studying RSM model can be accomplished by [42,44,45]:

1) Studying the response surface features (maximum and minimum location, and ridgelines).
2) Determining the area where the optimum response arises and obtaining a maximum or a minimum response.

The most common design for fitting the complete order polynomial model is Central Composite Design (CCD), which develops through a sequential investigation. If there is any evidence of lack of fit to fit data to the first order polynomial model, axial points can be generated in quadratic terms and with additional center points to develop CCD [44]. The CCD consists of the following three parts [46]:

1) A complete (or a fraction of) $2^k$ factorial or cube points, which is called the factorial points where $k$ is a number of factors.
2) Axial or star points that consist of $2k$ points set so that two points are chosen on the axis of each control factor at a distance of $\alpha$ from the center point (chosen as the point at the origin of the coordinates system). When $\alpha = 1$, the CCD is called faced CCD.
3) Center points $N_0$. 
Hence, the total general number of design points (n) in a CCD is [43,46]:

\[ n = \sum_{\text{cube points}} 2^k + \sum_{\text{star points}} 2^k + \sum_{\text{center points}} N_0 \]  

(1.3)

Figure 1.2 shows a CCD for \( k = 2, \alpha = \sqrt{2}, N_0 = 2 \) [46].

**Figure 1.2:** A CCD with two factors (a) The cube points part has factor levels (b) The axial points part at \((+\alpha, 0)\) \((-\alpha, 0)\) \((0, +\alpha)\) \((0, -\alpha)\), (c) The center points for cube and axial points parts at \((0,0)\), and (d) CCD design matrix with 10 design points

In CCD, the influences that can be predicted rely on the points type [42,43,46]:

1) The cube points can estimate the effect of linear and interaction (among factors), but not curvature effect in the response.
2) The center points can estimate curvature effect in the response, but not separate quadratic terms.
3) The star points can estimate quadratic terms.

In this study, a statistical analysis of the RSM numerically and graphically was conducted using Minitab software. The calculations in matrix form were accomplished by faced CCD design
where each RSM model was performed by detailed analysis (the number of factors and ranges) of each case study.

The main goal of this research is to propose a new efficient methodology to find the third generation of AHSS Through developing new DP steels by predicting and optimizing microstructure features to design the unique mechanical properties features at different strain rates. This new methodology consists of the multiscale material model for predicting the mechanical behavior of DP steels using simulated tensile test linking with the RSM model for providing the comprehensive statistical analysis. The multiscale material model is used to simulate the multiphase microstructure of DP steels and predict the flow stress of DP steels under quasi-static and dynamic loading conditions. Moreover, the comprehensive statistical parametric study and optimization were performed to investigate the influences and interactive interactions of microstructure parameters, such as ferrite and martensite grain size, volume fraction and morphology of martensite phase, and carbon content in DP steel, on the mechanical properties of DP steels.

This dissertation consists of the published (or submitted) papers in this research. The papers have been slightly revised for uniformity through the dissertation and references are moved to the end of the dissertation. In chapter two, micromechanical modeling of DP steels using 3D representative volume elements (3D RVEs) under quasi-static loading condition was proposed, which takes into account volume fraction and morphology of phases, chemical composition, and grain size. Numerical results from 3D RVE’s were then employed to perform a complete statistical analysis on the effect of various microstructure parameters on the energy absorption capacity of DP steels. The influences of ferrite grain size, volume fraction and grain size of martensite, and carbon content in DP steels on the tensile toughness were discussed in this chapter. Chapter three
and four focuses on using a full micro-macro multiscale material model using a dislocation density based nonlinear elastic-viscoplastic model coupled with RSM model for studying the effects of microstructure properties of DP steels on the DP steels mechanical behavior. The mean-field homogenization model (Digimat-MF) coupled with structural FEA (LS-DYNA) was adopted to accurately predict the mechanical behavior of DP steels under quasi-static and dynamic loading. That was followed by a systematic comprehensive statistical investigation by using RSM model for examining the impacts of microstructure parameters such as ferrite grain size, martensite volume fraction, and carbon content on the mechanical properties of DP steels under different strain rates as well as an evaluation of the effective microstructure parameters.
CHAPTER TWO: MICROSTRUCTURE OPTIMIZATION OF DUAL PHASE STEELS USING A REPRESENTATIVE VOLUME ELEMENT AND A RESPONSE SURFACE METHOD: PARAMETRIC STUDY

Dual phase (DP) steels have received widespread attention for their low density and high strength. This low density is of value to the automotive industry for the weight reduction it offers and the attendant fuel savings and emissions reductions. Recent studies on developing DP steels showed that the combination of strength/ductility could be significantly improved when changing the volume fraction and grain size of phases in the microstructure depending on microstructure properties. Consequently, DP steel manufacturers are interested in predicting microstructure properties and in optimizing microstructure design. In this work, a microstructure-based approach using representative volume elements (RVEs) was developed. The approach examined the flow behavior of DP steels using virtual tension tests with an RVE to identify specific mechanical properties. Microstructures with varied martensite and ferrite grain sizes, martensite volume fractions, carbon content, and morphologies were studied in 3D RVE approaches. The effect of these microstructure parameters on a combination of strength/ductility of DP steels was examined numerically using the finite element method by implementing a dislocation density-based elastic-plastic constitutive model, and a Response Surface Methodology (RSM) to determine the optimum conditions for a required combination of strength/ductility. The results from the numerical simulations are compared with experimental results found in the literature. The developed methodology proves to be a powerful tool for studying the effect and interaction of key microstructural parameters on strength and ductility and thus can be used to identify optimum microstructural conditions.
2.1 Introduction

2.1.1 Dual Phase (DP) steels

Advanced high strength steels (AHSS) offer the ability to produce stronger, safer, and lighter cars. To meet the demands of automobile manufacturers for these materials, steelmakers have developed new, low cost, high strength steels (HSS) and AHSS with superior strength and ductility [47]. In addition, they have developed a descriptive terminology for AHSS along with a number of different grades. These materials include the first generation AHSS with mainly ferrite-based microstructures and second generation AHSS with high manganese, austenitic-based microstructures. The first generation AHSS consist of transformation-induced plasticity (TRIP), DP, complex phase (CP), and martensitic (MART) steels [3]. The most important second generation austenitic AHSS grade is composed of twinning induced plasticity (TWIP) steels [6]. There is a growing need for third generation AHSS characterized by greater strength and formability than in first generation AHSS, and lower cost than that of the second generation AHSS. Efforts have been made to expand the range of first and second generation AHSS [3]. Demand is growing for stronger steel with lower mass, better stretchability (to improve formability), better crash energy management, reduced alloy requirements, and simpler manufacturing processes to reduce costs [48]. Dual phase steels have a range of strength and formability combinations depending on their microstructure. The microstructure of DP steels includes martensite phase particles dispersed in the soft ferritic matrix. Generally, DP steels contain a purely ferrite phase as a matrix with about a 3.3–47% fraction of martensite islands spread as a hard phase over a matrix [48].
2.1.2 Plastic deformation and work hardening behavior of DP steels

Flow stress of DP steels relies not solely on the characteristics of the ferrite and martensite phases but also on the volume fraction and morphology of the martensite phase [49–53]. During plastic deformation of DP steels, ferrite phase properties govern the yield behavior of DP steels, which is determined by the ferrite’s composition and grain size. The plastic deformation starts in the ferrite grain. Even though the martensite phase has a significant effect on strain hardening of DP steels, the martensite phase behavior generally shows elasticity unless deformation reaches high-stress levels [19,54,55]. In DP steels, the strength of the ferrite phase depends on the initial dislocation density resulting from compatible strains when the austenite phase alters into the martensite phase during cooling [56,57]. The martensite phase strength relies primarily on its carbon content, and its yield strength increases with increasing carbon content.

In DP steels, the transformation of the austenite phase to the martensite phase during cooling causes volume expansion. In turn, this volume increase initiates inelastic deformation. Hence, Geometrically Necessary Dislocations (GNDs) are formed at grain boundaries between ferrite and martensite phase to maintain lattice continuity in the adjacent ferrite grains that plastically deform. The number of the GNDs increases by increasing martensite volume fraction. Significant mobile dislocations that are amongst the GNDs can move instantly at the beginning of yielding behavior, resulting in a stress-strain curve that does show initial yield drop phenomenon [32,48,52,58].

2.1.3 The methodology

As alluded to previously, in order to increase safety and strength, automobile weight and overall performance, extraordinary strength materials with suitable combinations of strength and ductility are desired, such as that found in dual phase steels. DP steels demonstrate remarkable
mechanical properties, for instance, continuous work hardening behavior and an excellent energy absorption, besides the advantages of having decreased expense and a better formability compared to other AHSS grades. Therefore, steel makers attempt to improve the mechanical properties of DP steels by developing effective methodologies to determine the optimum DP microstructure leading to a maximum strength–ductility combination and identification of the effective microstructure parameters [2,32]. To that end, micromechanical modeling of DP steels coupled with a statistical tool can be utilized to create an efficient analytical model for determining the optimum mechanical properties of DP steels in terms of microstructure parameters: martensite volume fraction (MVF), martensite grain size (dm), ferrite grain size (df), and carbon content (C wt%) in DP steels.

A representative volume element (RVE) microstructure-based simulation approach is a methodology used to anticipate the flow stress of materials using their microscopic characteristics. RVE based techniques have been used by a number of authors as a general method for simulating and modeling the microstructure of DP steels [18,20–22,59–65]. These authors emphasize that 3D RVE techniques can predict the accurate flow stress of DP steels within the framework of continuum mechanics. Through the 3D RVE models, typically simplified microstructure characteristics are generated. However, 3D RVE models can be used to model more accurately the microstructures by including details that can be measured using 3D electron backscatter diffraction (EBSD) [18,65].

Understanding statistical arithmetical design basics, regression modeling methods, and optimization approaches are required to fit and identify from study data an appropriate response surface model. These methods are typically connected in RSM (a group of numerical and statistical techniques) to model and analyze DP microstructures where the combination of strength and
ductility are influenced by microstructure features (as different variables) in order to optimize this response [43]. Delincé et al. [66] developed a physical model for the work hardening behavior of DP steels to make a statistical investigation on the effect of martensite volume fraction, ferrite grain size, and carbon content on the flow stress of DP steels. Moreover, they provided through this model parametric study directions for developing the microstructures based on ferrite grain size, martensite volume fraction, and carbon content, toward differently formulated purposes regarding particular components mechanical properties, such as maximizing and characterizing the energy absorption or improving strength with flexibility. Nevertheless, most of the previous studies [2,23,27,32,50,52,53,55,64,66–68] on microstructure based micromechanical models of DP steels and the optimization of its microstructure characteristics have only included a few microstructure features such as martensite volume fraction and ferrite grain size in their models and without performing any numerical or statistical study. Details of previous studies on the micromechanical model and microstructural design optimization that have been carried out on DP steels are provided in Table 2.1. It can be seen in Table 2.1 that previous research works on the parametric study of a microstructure-based micromechanical model of DP steels did not show the effects of interactions between the microstructural parameters on the combination of high strength and ductility and the optimization of its microstructure characteristics. Thus, the effects of interactions between the microstructural parameters on the performance of DP steels are still outstanding as well as microstructural parameter optimization. Furthermore, the previous research works were performed employing the simplistic approach of modifying one parameter at a time while maintaining the other parameters fixed.
Table 2.1: Finite element model studies, based on the micromechanical model of DP steels and
the optimization of its microstructure characteristics were conducted.

<table>
<thead>
<tr>
<th>No.</th>
<th>Author</th>
<th>Microstructure Parameters</th>
<th>Methodology</th>
<th>Finding</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Jiang et al. [50]</td>
<td>MVF, $d_m$, and $d_f$</td>
<td>A theoretical model based on Ashby strain hardening theory was used. RVE or RSM were not used.</td>
<td>The effect of $d_f$ on the flow stress of DP steels was found to obey the Hall-Petch relationship. Flow stress and strain hardening were controlled by MVF at low strains and only barely controlled at high strains.</td>
</tr>
<tr>
<td>2</td>
<td>Balliger et al. [52]</td>
<td>MVF and $d_m$</td>
<td>A theoretical model based on the Ashby strain hardening theory was used. RVE and RSM were not used.</td>
<td>The work-hardening rate of DP steels is dependent on $\sqrt{\frac{MVF}{d_m}}$.</td>
</tr>
<tr>
<td>3</td>
<td>Sun et al. [53]</td>
<td>MVF, $d_m$, and $d_r$</td>
<td>A 2D RVE micromechanical model for the actual microstructures of DP steels was used in 2D FEA. RVE and RSM were not used.</td>
<td>The model was in good agreement with experimental observations. 2D RVE statistically represented $d_r$, $d_m$, and MVF in DP steels.</td>
</tr>
<tr>
<td>4</td>
<td>Sodjit et al. [32]</td>
<td>MVF, $d_m$, and $d_f$</td>
<td>A 2D RVE micromechanical model for the actual microstructures of DP steels was used in 2D FEA. RVE and RSM were not used.</td>
<td>The flow stress of DP steels was strongly affected by the morphology of the dispersed martensite phase.</td>
</tr>
<tr>
<td>5</td>
<td>Amirmaleki et al. [2]</td>
<td>$d_m$, and MVF</td>
<td>The 3D RVE micromechanical model was used. RSM was not used.</td>
<td>The ultimate tensile stress of DP steels with less than 0.5% error was predicted.</td>
</tr>
<tr>
<td>6</td>
<td>Uthaisangsuk et al. [64]</td>
<td>MVF, C wt%</td>
<td>The 3D RVE micromechanical model was used. RSM was not used.</td>
<td>The authors suggested that understanding the interactions between microstructure properties and mechanical properties of the individual phases would provide steel and automotive manufacturers with a methodology for creating desired microstructures and optimizing DP steels.</td>
</tr>
<tr>
<td>7</td>
<td>Delincé et al. [66]</td>
<td>$d_f$ and MVF</td>
<td>A physical model based on an evolution law for the ferrite–ferrite grain boundary dislocations (GBD) including saturation as well as the contribution of the back stress linked to the GBD was employed. RVE and RSM were not used.</td>
<td>The model was used to generate a parametric study on the influence of $d_f$, MVF, and C wt% content on the plastic behavior of DP steels. Non-trivial optima in the strength of DP steels are found for intermediate MVF, depending on the $d_f$ and the C wt% content.</td>
</tr>
<tr>
<td>8</td>
<td>Jafari et al. [67]</td>
<td>MVF, $d_m$, and $d_f$</td>
<td>A dislocation density and a damage model besides an elastic-plastic model for grain boundaries were employed. A Voronoi tessellation technique was applied to generate the microstructures of the DP steels. RVE and RSM were not used.</td>
<td>A parametric study to examine the effects of microscopic factors on the flow stress of DP steels. The research showed that $d_f$, $d_m$, and MVF play a significant role in the flow stress of DP steels. They noticed that for intermediate grain sizes the toughness of DP steels would be optimized.</td>
</tr>
<tr>
<td>No.</td>
<td>Author</td>
<td>Microstructure Parameters</td>
<td>Methodology</td>
<td>Finding</td>
</tr>
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<td>-------------</td>
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</tr>
<tr>
<td>9</td>
<td>Krajewski and Nowacki [23]</td>
<td>MVF, alloying elements, heat treatment conditions</td>
<td>An artificial neural network was used to model the relationships of DP chemical compositions and properties.</td>
<td>The model allows estimation of the effects of MVF, alloying elements, and heat treatment conditions on the mechanical properties of DP Steels.</td>
</tr>
<tr>
<td>10</td>
<td>S. K. Paul [68]</td>
<td>MVF</td>
<td>The influence of MVF on the tensile properties of DP steels was investigated using finite element simulation on the RVE of DP steel microstructures.</td>
<td>Ductility decreased and ultimate tensile stress increased with increasing martensite volume fraction in DP steel.</td>
</tr>
<tr>
<td>11</td>
<td>S. K. Paul [27]</td>
<td>MVF and d_\text{f}</td>
<td>The flow stress and plastic strain localization in DP 590 steel were studied utilizing a microscope-based approach with 2D and 3D RVE.</td>
<td>Flow stress of DP steels was strongly affected by the morphology of the dispersed the martensite phase.</td>
</tr>
</tbody>
</table>

This methodology requires numerous experimental and computational work, which is both costly and time-consuming. In addition, this simple method is not capable of investigating the effects of interaction between microstructural parameters and cannot be used to perform experimental optimization.

The current study aims to examine the influences of microstructure parameters, namely: martensite volume fraction (MVF), martensite grain size (d_m), ferrite grain size (d_f), and carbon content (C wt%) on the flow stress of DP steels. A 3D micromechanical model is developed to accurately predict the flow behavior of DP steels in uniaxial tension. The simulation is then utilized to perform a parametric study on the effect of various microstructure parameters on plastic behavior. Specifically, the current study investigates the effect of microstructure parameters (MVF, d_m, d_f, and carbon content (C wt%)) in DP steels on the combination of strength and ductility of DP steels. The 3D RVE model that can precisely predict the flow stress of DP steels under uniaxial loading condition is developed, and the model is then used to generate a parametric study on the effect of microscale parameters on the inelastic behavior. This is followed by a systematic RSM investigation of the influences of microscope parameters on the flow stress of DP steels as well as an evaluation of the effective microscopic parameters. In addition, the optimum
values of microstructure parameters are derived for achieving the maximum strength as well as highest ductility.

### 2.2 Micromechanical modeling

The microscope features of DP steels that can be considered on different levels and length scales cause this remarkable strength and ductility combination. The crystalline structure in each phase affects on the flow stress of DP steels such as ductility and strength. Defects such as dislocations exist naturally and may be controlled to cause great differences in the flow stress of DP steels. At the crystalline structure level, the type, distribution, size, volume fraction and orientation of grains for each phase affect on the flow stress of DP steels [59]. Microstructure models are generally used in order to understand the local mechanism of each phase and mechanisms controlling the continuum elastic–plastic behavior of heterogeneous materials such as DP steels. Different scale modeling and approaches for micromechanical modeling of DP steels, which takes into account volume fraction and morphology of phases, chemical composition, and grain size are summarized by Tasan et al. [24]. There are three basic features of a micromechanical model for a general multiphase material:

1) Geometry dimensions of RVE that represents the essential characteristics of the microstructure.

2) The constitutive equations that describe the flow stress of each phase and the grains boundaries if applicable.

3) A homogenization scheme that correlates the microscopic behavior of material to its macroscopic behavior depending on the mechanical behavior of the RVE [2,59].

In general, a RVE should have the general features of the entire microscopic characteristics such as volume fraction, morphology, and the random phases. For micromechanical simulation of
multi-phase materials, the RVE is part of a methodology comprising four components as shown in Figure 2.1.

A basic cell model can define a simple 2D or 3D RVE, or it can be more complex by using a real microstructure. Recently, several researchers have generated 2D and 3D RVEs based on simplified and real microstructure features [2,24,27,32,51,59,63,64,69–71]. Mori–Tanaka’s assumption is the straightforward hypothesis to create a 3D RVE of a multi-phase material [71]. In this assumption, the hard phase material represents inclusions that are spread in a matrix representing the soft phase material. For instance, 3D RVE of DP steels that consider the ferrite phase as the matrix and the martensite phase as an inclusion were created by, Amirmaleki et al. [2], Ramazani et al. [63] Uthaisangsuk et al. [64], and Paul [70]. The volume fraction of phases was represented according to the number of elements in FE for each phase.

2.2.1 Generation of 3D RVE

In previous work [2,63,64,70] on 3D RVEs of DP steels based on real microstructures, 3D micromechanical modeling results produced more accurate flow curves than 2D modeling. Also, in their research, the martensite islands were disseminated at random in the 3D RVE irrespective of its morphology, and the ellipsoid shape with aspect ratios of 1.87 and 1.78 was the most similar inclusion shape to embody the martensite phase.

The size of the RVE should be carefully selected. A too small RVE cannot represent the average characteristics of the whole microstructure and a too large RVE significantly increases the complexity and time of calculations. For these reasons, an adapted size for RVE is automatically calculated by Digimat, which takes into account the following points:
Figure 2.1: The micromechanical modeling stages.

- At least 3 to 5 inclusions can be placed along each of the three axes of the RVE.
- The size and the shape of each inclusion phase.
- The orientation of each inclusion phase.

In this study, 3D RVEs were generated by Digimat-FE software where the martensite islands were designed as inclusions and ferrite phase as the matrix in DP steels. The martensite islands were simulated as the ellipsoid model, and the size and aspect ratio of the martensite islands were both defined through the model. In addition, the martensite volume fraction and its morphology were counted for producing a 3D RVE that was more demonstrative of the real microscope features of DP steels. As can be seen in Figure 2.2, after defining morphological features of DP steel microstructures, Digimat generates a random 3D RVE and provides
information about the phase data, the effective volume fraction of the martensite islands, and their numbers in the 3D RVE.

<table>
<thead>
<tr>
<th>Phase information</th>
<th>Hard phase (Inclusions)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of inclusions</td>
<td>Effective volume fraction</td>
</tr>
<tr>
<td>127</td>
<td>14.27%</td>
</tr>
</tbody>
</table>

**Figure 2.2:** 3D RVE generation for MVF 14% (a) martensite phase information and (b) RVE

Moreover, Digimat automatically calculates a tailored size for the RVE where at least 3 to 5 inclusions can be positioned along each of the three axes of the RVE or can be manually defined via three axes of the RVE. Next, the inclusions and the surrounding matrix are meshed into finite elements. The element types that are used are solid brick elements with four integration points as shown in Figure 2.3. The mesh density can be specified with the number of elements along each of three axes of the RVE.
2.2.2 Constitutive equations description

In the 3D micromechanical model, the constitutive equations of each phase are needed in order to investigate deformation behavior of DP steel. In the current study, the elastic modulus for ferrite and martensite was assumed to be 210 GPa [2]. In the micromechanical finite element model, von Mises yield, associative flow, and isotropic hardening rule are utilized for each particular phase. The dislocation density model that was formulated by Rodriguez and Gutierrez [72] was used by several studies [2,25,26,51,63,64,70,73–75].

This dislocation-based model was used to describe the flow stress for each single phase where the typical relationship between the dislocation density and flow stress can be written as:
\[ \sigma_{flow} = \sigma_0 + \Delta \sigma_c + \Delta \sigma = \sigma_0 + \Delta \sigma_c + \alpha M \mu b \sqrt{\rho} \] (2.1)

where \( \alpha \) is a constant, \( M \) is the Taylor factor, \( \mu \) is the shear modulus, \( b \) is the Burger’s vector, and \( \rho \) is the dislocation density. The first term in Eq (2.1) is the contribution of the stress friction, Peierls stress, and effects of alloying elements in solid solution that are supposed to be uniformly scattered in each phase, and it can be described as [2,51,64,70]:

\[
\sigma_0 \text{ (in MPa)} = 77 + 80\% \text{Mn} + 750\% \text{P} + 60\% \text{Si} + 80\% \text{Cu} + 45\% \text{Ni} \\
+ 60\% \text{Cr} + 11\% \text{Mo} + 5000\% \text{N} \tag{2.2}
\]

The second term in Eq (2.1) represents precipitation hardening based on carbon content in solid solution. In the case of ferrite, it is [2,51,70]:

\[
\Delta \sigma_c^f = 5000 \times \% \text{C}_{ss}^f \tag{2.3}
\]

in the case of martensite, it is expressed by [3,6,47]:

\[
\Delta \sigma_c^m = 3065 \times \% \text{C}_{ss}^m - 161 \tag{2.4}
\]

where \% \text{C}_{ss}^f \ and \% \text{C}_{ss}^m \ is the wt.% carbon content in solid solution in ferrite and martensite, respectively. The carbon content in the ferrite phase is assumed to be 0.02%, which is the solubility limit for carbon in ferrite at room temperature. Even though the increase of the flow and tensile strengths with increasing martensite volume fractions at a defined carbon content in the martensite phase is noted and broadly reported (e.g. [50,76], to cite only a few), the law of mixture can be used to calculate the carbon content in the martensite phase based on the carbon content in DP steel [76]. It can be described as:

\[
\% \text{C}_{ss}^{DP} = \% \text{C}_{ss}^f \times \text{FVF} + \% \text{C}_{ss}^m \times \text{MVF} \tag{2.5}
\]

where \% \text{C}_{ss}^{DP} \ is the nominal carbon composition of the DP steel, and FVF and MVF are the ferrite volume fraction and martensite volume fraction, respectively. This is just a simplifying, but it is considered as a reasonably suitable approximation.
The third term in Eq (2.1) is the Taylor Evolution Law. According to the Mecking-Kocks theory, the rate of dislocation density evolution to shear strain during the deformation is the result of the competition between the rate of production of dislocation and the annihilation rate of dislocation \([75]\), which can be written as:

\[
\frac{d\rho}{dy} = \left[ \frac{d\rho}{dy} \right]_{\text{stored}} + \left[ \frac{d\rho}{dy} \right]_{\text{recovery}} = \frac{1}{bL} - k_r \rho
\]  

(2.6)

where \(L\) is the dislocation mean free path and \(k_r\) is a constant. Rodriguez and Gutierrez \([72]\) further developed this concept for the ferritic and martensitic phase; thus, the effective stress-strain relation is given by:

\[
\Delta \sigma = \alpha M \mu \sqrt{b} \sqrt{\frac{1 - \exp(-M k_r \varepsilon)}{k_r L}}
\]  

(2.7)

Once the description of the three terms in Eq (1) has been defined, the complete methodology for defining the flow stress of each phase in the DP steel is:

\[
\sigma_{\text{flow}} = \sigma_0 + \Delta \sigma_c + \alpha M \mu \sqrt{b} \sqrt{\frac{1 - \exp(-M k_r \varepsilon)}{k_r L}}
\]  

(2.8)

where \(\sigma_{\text{flow}}\) and \(\varepsilon\) are responsible for the true flow stress (von Mises stress) and true strain, respectively. The parameter values that are used for the ferrite and martensite phases in 3D RVE simulation are listed in Table 2.2 for each phase.
Table 2.2: Model parameters for Eq (2.8)

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Ferrite</th>
<th>Martensite</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>M (Taylor factor)</td>
<td></td>
<td>3</td>
<td></td>
</tr>
<tr>
<td>b (Burger’s vector)</td>
<td>2.5x10^{-10} m</td>
<td></td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>μ (Shear modulus)</td>
<td>80,000 MPa</td>
<td></td>
<td></td>
</tr>
<tr>
<td>α (Constant)</td>
<td>0.33</td>
<td></td>
<td></td>
</tr>
<tr>
<td>L (Dislocation mean free path)</td>
<td>d_f</td>
<td>3.8x10^{-8} m</td>
<td></td>
</tr>
<tr>
<td>k_r (Recovery rate)</td>
<td>10^{-5}/d_f</td>
<td>41</td>
<td></td>
</tr>
</tbody>
</table>

2.2.3 Load and boundary conditions application

Appropriate load and boundary conditions should be used in a 3D RVE so as to correctly foresee the deformation behavior of DP steel in a certain condition. Several studies reported that applying periodic boundary conditions to simulate the DP steel microstructure is more accurate than other boundary condition techniques such as prescribed displacement and prescribed traction boundary conditions [2,51,63,64,70,74,77]. Given that, the periodic boundary condition is used to provide a better approximation of the general microstructure properties of DP steel. A general form of the periodic boundary condition is described as:

\[
\vec{x}^\pm = F_M \times (\vec{x}^\pm) + \vec{x}^0
\]

where \( F_M \) is the deformation gradient tensor that represents the deformed configuration of RVE in a point with initial position vector \( \vec{x} \) at reference configuration \( V_0 \) and the current position vector \( \vec{x} \) at current configuration \( V \) [77]. For the RVE shown in Figure 2.4, the periodic boundary condition is written as follows:

\[
\begin{align*}
\vec{x}_T &= \vec{x}_B + \vec{x}_4 - \vec{x}_1 \\
\vec{x}_R &= \vec{x}_L + \vec{x}_2 - \vec{x}_1 \\
\vec{x}_3 &= \vec{x}_2 + \vec{x}_4 - \vec{x}_1
\end{align*}
\]
where $\mathbf{x}_R$, $\mathbf{x}_L$, $\mathbf{x}_T$, and $\mathbf{x}_B$ represent the position vectors at the right, left, top and bottom of the RVE boundary condition, respectively. $\mathbf{x}_i$ (i=1,2,3, and 4) represents position vectors of the corner points in the current configuration, respectively, and can be described by $F_M$:

$$\mathbf{x}_i = F_M \cdot \mathbf{x}_i, \quad i = 1,2,3,4 \text{ with } \mathbf{x}_i \text{ on } \Gamma_0 \text{ and } \mathbf{x}_i \text{ on } \Gamma$$

(2.11)

where $\Gamma_0$ and $\Gamma$ are initial and current RVE boundaries, respectively.

![Figure 2.4: A typical 2D RVE diagram](image)

2.2.4 Homogenization technique

To investigate the macroscopic behavior of multi-phase materials, different homogenization approaches are usually utilized. These homogenization schemes provide flexible approaches to estimate micro-macro structure-property relations for multi-phase materials for which other techniques cannot predict the collective behavior of the multi-phase structure. DP steel is considered a heterogeneous material whose microstructure consists of a matrix material, ferrite phase, and multi-phases of a so-called “inclusion,” martensite phase. First-order computational homogenization technique becomes a powerful approach for estimating the continuum mechanical behavior of non-linear multi-phase materials [2,51,63,64,70,74,77]. This technique is conducted in three stages as shown in Figure 2.5:
1) The deformation gradient tensor $F_M$ is computed for every integration point of the macroscopic mesh in the RVE model.

2) $F_M$ is employed to define the boundary conditions to be applied on the RVE that is specified to this point.

3) An average of the RVE stress field response over the volume of the RVE determines the macroscopic stress tensor $P_M$ based on the solution of the boundary value problem of the RVE.

Thus, the flow stress at the macroscale level is obtainable. Moreover, the local macroscale consistent tangent is obtained from the microstructural stiffness as shown in Figure 2.5.

![Figure 2.5: First order computational homogenization scheme](image-url)
2.3 Response Surface Methodology (RSM)

RSM is a statistical design of experimental technique, which refers to the method of arranging the tests so that the appropriate data can be examined statistically [78]. RSM is employed to examine the relationship between a response variable and a set of factors. RSM was initially created to fit the model of physical experiments by Box and Draper [78] and later implemented across other topics. The RSM implementation is summarized in Figure 2.6.

In this study, RSM was employed to determine the required points of analysis (the 3D RVE modeling) within specified ranges of microstructure parameters: a \(d_f\) range of 0.7 – 13 \(\mu\text{m}\), a \(d_m\) range of 0.56 – 1.4 \(\mu\text{m}\), a C wt\% range of 0.034 – 0.23 wt\%, and a MVF range of 3.3 – 47\% in DP steels. The ranges of microstructure parameters \((d_f, d_m, C \text{ wt\%} \text{ and MVF})\) were estimated based on the previous literature review and few preliminary trials. The micromechanical modeling was conducted according to the simulation points in the design matrix obtained from RSM. This RSM model initially allowed us to design the experiment effectively, and, after that, provided data for parametric study and optimization.

![Diagram](Diagram_2.6.png)

**Figure 2.6**: The steps taken in creating an RSM model
The design of the investigation matrix depending on the Central Composite approach was generated, using MINITAB software after the design parameters and their ranges had been introduced. The complete quadratic polynomial regression model as shown in Eq (2.12) was determined for foretelling the response variable \( F \), that is toughness, in terms of the independent variables \( X_1, X_2, X_3, X_4 \), that are the microstructure parameters. Subsequently, the 3D RVE modeling was carried out according to the designed analysis matrix listed in Table 2.3 which was obtained by the RSM model using MINITAB software.

\[
F = a_0 + a_1X_1 + a_2X_2 + a_3X_3 + a_4X_4 + a_{11}X_1^2 + a_{22}X_2^2 + a_{33}X_3^2 + a_{44}X_4^2 + a_{12}X_1X_2 + a_{13}X_1X_3 + a_{14}X_1X_4 + a_{23}X_2X_3 + a_{24}X_2X_4 + a_{34}X_3X_4
\]  

(2.12)

Thereafter, the 3D RVE micromechanical model of DP steels was performed, and toughness was then introduced into the previously designed matrix. Toughness, in general, is the capability of materials to absorb energy in operation before separating and to deform inelastically. The toughness is the key to determine a good strength/ductility combination.

The toughness is the strong indication to determine a good strength/ductility combination. A good toughness means a high strength and a high ductility, and vice versa [79]. Material toughness is measured by computing the area under the stress-strain curve for tensile test, and it is expressed in tensile toughness (energy unit/volume unit).

When the RSM model is run and investigated, the results are presented in the form of 3D and 2D diagrams. These charts exhibit how the response variable, toughness, is a function of four parameters based on a model regression as shown in Eq (2.12). In a 2D chart, the RSM is viewed as a 2D contour plot where all data that have the same response are attached to create contour lines of constant responses. A 3D chart illustrates a 3D view that may provide a clearer understanding.
of the RSM. Moreover, the microstructure parameters optimization is performed, and corresponding microstructure characteristics are estimated.

Table 2.3: Design of analysis matrix using MINITAB software

<table>
<thead>
<tr>
<th>Design Points (Run order)</th>
<th>Microstructure Parameters</th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>d (µm)</td>
<td>d_m (µm)</td>
<td>MVF (%)</td>
<td>C wt%</td>
</tr>
<tr>
<td>DP#1</td>
<td>3.775</td>
<td>0.725</td>
<td>14.23</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#2</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#3</td>
<td>9.925</td>
<td>0.725</td>
<td>14.23</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#4</td>
<td>9.925</td>
<td>1.175</td>
<td>36.075</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#5</td>
<td>3.775</td>
<td>1.175</td>
<td>14.23</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#6</td>
<td>9.925</td>
<td>0.725</td>
<td>36.075</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#7</td>
<td>9.925</td>
<td>1.175</td>
<td>14.23</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#8</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#9</td>
<td>3.775</td>
<td>0.725</td>
<td>36.075</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#10</td>
<td>3.775</td>
<td>1.175</td>
<td>36.075</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#11</td>
<td>9.925</td>
<td>0.725</td>
<td>14.23</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#12</td>
<td>3.775</td>
<td>1.175</td>
<td>14.23</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#13</td>
<td>9.925</td>
<td>1.175</td>
<td>36.075</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#14</td>
<td>9.925</td>
<td>1.175</td>
<td>14.23</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#15</td>
<td>3.775</td>
<td>1.175</td>
<td>36.075</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#16</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#17</td>
<td>3.775</td>
<td>0.725</td>
<td>14.23</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#18</td>
<td>9.925</td>
<td>0.725</td>
<td>36.075</td>
<td>0.1783</td>
</tr>
<tr>
<td>DP#19</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#20</td>
<td>3.775</td>
<td>0.725</td>
<td>36.075</td>
<td>0.0748</td>
</tr>
<tr>
<td>DP#21</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#22</td>
<td>6.850</td>
<td>0.95</td>
<td>3.3</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#23</td>
<td>6.850</td>
<td>0.95</td>
<td>47</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#24</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.023</td>
</tr>
<tr>
<td>DP#25</td>
<td>6.850</td>
<td>0.5</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#26</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.230</td>
</tr>
<tr>
<td>DP#27</td>
<td>6.850</td>
<td>1.4</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#28</td>
<td>6.850</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#29</td>
<td>0.7</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
<tr>
<td>DP#30</td>
<td>13</td>
<td>0.95</td>
<td>25.15</td>
<td>0.1265</td>
</tr>
</tbody>
</table>

2.4 The 3D RVE modeling Procedure of DP Steels

In this study, 3D RVE modeling was conducted to obtain flow behavior of DP steels, which are considered composite materials consisting of martensite islands as inclusions and a ferrite phase matrix as mentioned in section 2.2.2. The whole simulation procedure was performed using
MINITAB, OriginLab, and Digimat software. The 3D RVE modeling of the flow behavior of DP steels was implemented in six steps: (1) An analysis matrix that contains design points was designed and created using Minitab as mentioned in section 3. (2) Flow curves of two phases for each design point (30 total design points) were determined using OriginLab. (3) Flow curves of two phases for each design point were introduced to Digimat-FE. (4) 3D RVEs for each design point were generated, and loading and boundary conditions were defined in Digimat-FE as mentioned in sections 2.2.2, 2.2.3, and 2.2.4 (5) The flow curve of the 3D RVE for each design point in Digimat-FE was obtained, and toughness was calculated for each flow curve using OriginLab. (6) Analysis of the RSM model by adding toughness for each design point to the design of the analysis matrix was completed to obtain 2D contour plots, 3D surface plots, and the microstructure parameters optimization.

An appropriate flow behavior of the ferrite and martensite phases in the 3D RVE model were determined according to Eq (2.8) and the required parameters that are listed in Table 2.3. The work hardening behavior of constituents was assumed to follow the power law equation [53].

$$
\sigma = \sigma_y + K \varepsilon_p^n
$$

(2.13)

where $\sigma$ is the flow stress, $\sigma_y$ is the initial yield strengths, $\varepsilon_p$ is the plastic strain, $K$ is the hardening modulus, and $n$ is the hardening exponent. Thus, the OriginLab software was conducted to fit the Ludwik power law equation to the analytical flow stress of ferrite and martensite phase to define mechanical constant (K,n) of constituents for all design points. What follows in Table 2.4 and Figure 2.7 is an example of these implementation of the Curve Fitting application in OriginLab software for design points (1), (2), and (3) to determine Hardening exponent ($n$) and modulus ($K$).
2.5 Results and discussion

In this study, the periodic boundary condition was applied as mentioned in section 2.2.3. All the simulation points were applied under static tension load condition and the peak strain value (0.14) at the onset of necking.

Table 2.4: The analytical and fitted flow stress of DP steel constituents for design points (1), (18), and (29).

<table>
<thead>
<tr>
<th>Design Points (Run order)</th>
<th>Flow stress according to Eq (2.8)</th>
<th>Flow stress according to fitted power law equation Eq (2.13)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DP#1</td>
<td>$\sigma_{flow}^f = 337 + 1.25 \times \sqrt{(1 - EXP(-7.947\varepsilon)/(10^{-5})}$</td>
<td>$\sigma_{flow}^f = 386.7 + 861\varepsilon^{0.562}$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_{flow}^m = 1268.4 + 1.25 \times \sqrt{(1 - EXP(-123\varepsilon)/(1.56 \times 10^{-6})}$</td>
<td>$\sigma_{flow}^m = 1736.9 + 3356.5\varepsilon^{0.103}$</td>
</tr>
<tr>
<td>DP#18</td>
<td>$\sigma_{flow}^f = 337 + 1.25 \times \sqrt{(1 - EXP(-3.023\varepsilon)/(10^{-5})}$</td>
<td>$\sigma_{flow}^f = 367.7 + 735\varepsilon^{0.629}$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_{flow}^m = 1459.5 + 1.25 \times \sqrt{(1 - EXP(-123\varepsilon)/(1.56 \times 10^{-6})}$</td>
<td>$\sigma_{flow}^m = 1928 + 3713.4\varepsilon^{0.1047}$</td>
</tr>
<tr>
<td>DP#29</td>
<td>$\sigma_{flow}^f = 337 + 1.25 \times \sqrt{(1 - EXP(-42.86\varepsilon)/(10^{-5})}$</td>
<td>$\sigma_{flow}^f = 450.4 + 1728\varepsilon^{0.6}$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_{flow}^m = 1405.6 + 1.25 \times \sqrt{(1 - EXP(-123\varepsilon)/(1.56 \times 10^{-6})}$</td>
<td>$\sigma_{flow}^m = 1874.02 + 3409\varepsilon^{0.09294}$</td>
</tr>
</tbody>
</table>

Figure 2.7: The analytical and fitted stress-strain curves of DP steel constituents for design points (1) using OriginLab software (a) ferrite phase and (b) martensite phase

The results of the 3D RVE modeling of DP steels microstructure characteristics and the RSM model are discussed in this section. The effects and interactions of microstructure parameters with the toughness of DP steels were investigated to optimize microscopic parameters. To estimate
the accuracy of the 3D RVE simulation results, the experimental data that contained statistical quantitative metallography and the stress-strain curve of DP500 [2] were compared to the predicted numerical stress-strain curves at three different techniques of grain size distribution as shown in Figure 2.8. Figure 2.9 and Table 2.5 show the analytical and fitted flow curves to obtain mechanical constant (K,n) for constituents of DP500.

**Figure 2.8:** Comparison between the experimental and numerical results at three different techniques of martensite grain size distribution in the generated 3D RVE

**Table 2.5:** The analytical and fitted flow stress for constituents of DP500

<table>
<thead>
<tr>
<th>Exp. Data</th>
<th>Flow stress according to Eq (2.8)</th>
<th>Flow stress according to fitted power law equation Eq(2.13)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DP500</td>
<td>$\sigma_{flow}^f = 327 + 1.25 \times \sqrt{1 - EXP(-5.51e)/(10^{-5})}$</td>
<td>$\sigma_{flow}^f = 337 + 725e^{0.449}$</td>
</tr>
<tr>
<td></td>
<td>$\sigma_{flow}^m = 1420.25 + 1.25 \times \sqrt{1 - EXP(-123e)/(1.56 \times 10^{-6})}$</td>
<td>$\sigma_{flow}^m = 1529 + 3541.63e^{0.0896}$</td>
</tr>
</tbody>
</table>
Figure 2.9: The analytical and fitted stress-strain curves of (a) ferrite and (b) martensite in DP500 steel

As can be seen in Figure 2.8, more accurate results are achieved when actual grain size distribution is used; however, the uniform and fixed grain distribution achieve acceptable accuracy with 2% to 4% error.

2.5.1 FE simulation of the 3D RVE

In this study, the ferrite grain size (df), the martensite grain size (dm), the martensite volume fraction (MVF) and its morphology (shape), and carbon content (C wt%) were considered in order to model the 3D RVE for all design points in the analysis matrix presented in Table 2.3. Furthermore, ellipsoidal shapes are used to represent martensite islands. For simplification, the fixed grain distribution and average aspect ratio were considered. All of this data was entered into the Digimat software to create the 3D RVEs for all design points. Table 2.6 shows a sample of 3D RVEs for design points (1), (10), and (22) in the RSM matrix.

Figure 2.10 shows samples of the flow curves of the composite (DP steel), ferrite, and martensite for some design points (PD#1, PD#10, and PD#22) in the analysis design matrix. The equivalent von Mises stress and plastic strain distribution at $\varepsilon = 0.14$ in the 3D RVEs for some design points (DP#1, DP#10, and DP#22) in the analysis design matrix are presented in Table 2.7.
**Table 2.6**: Specification of the generated 3D RVE’s samples for design point (1), (10), and (22) in the RSM matrix

<table>
<thead>
<tr>
<th>#</th>
<th>MP</th>
<th>RVE</th>
<th>RVE mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
</tr>
<tr>
<td>1</td>
<td></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td>10</td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
<td><img src="image7.png" alt="Image" /></td>
</tr>
<tr>
<td>22</td>
<td><img src="image8.png" alt="Image" /></td>
<td><img src="image9.png" alt="Image" /></td>
<td><img src="image10.png" alt="Image" /></td>
</tr>
<tr>
<td></td>
<td></td>
<td><img src="image11.png" alt="Image" /></td>
<td><img src="image12.png" alt="Image" /></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>d_f</th>
<th>d_m</th>
<th>MVF</th>
<th>C wt%</th>
<th>Data</th>
<th>Inclusions Number:</th>
<th>Effective MVF:</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.78</td>
<td>0.73</td>
<td>14.2</td>
<td>0.075</td>
<td></td>
<td>127</td>
<td>14.3%</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>3.775</td>
<td>1.75</td>
<td>36.08</td>
<td>0.075</td>
<td></td>
<td>362</td>
<td>36.06%</td>
</tr>
<tr>
<td>22</td>
<td>6.85</td>
<td>0.95</td>
<td>3.3</td>
<td>0.127</td>
<td></td>
<td>27</td>
<td>3.32%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th>No. of elements</th>
<th>Effective MVF</th>
<th>Total No. of elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Inclusions</td>
<td>3814</td>
<td>14.13%</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Matrix</td>
<td>23186</td>
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</tr>
<tr>
<td>10</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Inclusions</td>
<td>9637</td>
<td>35.69%</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
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<td>Matrix</td>
<td>17363</td>
<td>64.31%</td>
</tr>
<tr>
<td>22</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Inclusions</td>
<td>886</td>
<td>3.3%</td>
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<td></td>
<td></td>
<td></td>
<td>Matrix</td>
<td>26114</td>
<td>96.7%</td>
</tr>
</tbody>
</table>

= Ferrite + Martensite
Figure 2.10: Numerical true stress-strain curves of DP steels and their constituents for (a) design point (1), (b) design point (10), and (c) design point (22)

It can be seen in Figure 2.10 and Table 2.7 that the martensite phase is accountable for strengthening the DP steels and the ferrite phase is accountable for the plastic behavior. In some design points, the martensite phase generally exhibited elastic behavior or some levels of plastic behavior. In general, the martensite strength can be expressed as an aggregate of various strengthening mechanisms such as the effect of the carbon content, the grain size, the contribution
of the alloying elements, the effect of the dislocations, and the carbide particles [72]; however, the strength of the ferrite phase depends on the ferrite grain size and the martensite volume fraction.

**Table 2.7**: Distribution of equivalent von Mises and plastic strain at $\varepsilon = 0.14$ for design point (1), (10) and (22) in the RSM matrix.

<table>
<thead>
<tr>
<th>DP#</th>
<th>Distribution of equivalent von Mises</th>
<th>Distribution of plastic strain</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td><img src="" alt="Image" /></td>
<td><img src="" alt="Image" /></td>
</tr>
<tr>
<td>10</td>
<td><img src="" alt="Image" /></td>
<td><img src="" alt="Image" /></td>
</tr>
<tr>
<td>22</td>
<td><img src="" alt="Image" /></td>
<td><img src="" alt="Image" /></td>
</tr>
</tbody>
</table>
It can be seen in Table 2.7 through the distribution of plastic strain that during inelastic behavior, the ferrite phase tends to deform plastically; however, the majority of martensite phase shows elastic behavior and which limits further plastic deformation of the ferrite phase. Thus, the strain hardening increases at the ferrite-martensite grain boundary and produces localized inelastic deformation.

The localized deformation occurs because of dislocation generation within the ferrite phase. These dislocations move toward the grain boundary within the ferrite grain, and, at the ferrite-martensite interface, the dislocations prevent further movement, causing dislocations to accumulate at the interface. Hence, more martensite islands (MVF) in the microstructure cause more interface areas between ferrite and martensite grains that lead to more localized deformation and high strain hardening as shown in design point (10) in Table 2.7.

In order to estimate the accuracy of the RSM modeling results, a simple sensitivity analysis was carried out to investigate the effect of changing microstructure parameters on the flow stress of DP steels. Consequently, the effect of each microstructure parameter on the flow stress of DP steels is achieved by changing the values of this individual microstructure parameter while keeping the values of all other parameters constant as shown in Figure 2.11.

As can be seen in Figure 2.11, the microstructure parameters that have the most influence on the flow stress of DP steels are the martensite volume fraction (MVF) and ferrite grain size (df). However, the minor effect on the flow stress is found in the martensite grain size (dm) and the carbon content (C wt%) in DP steel. Overall, increasing each microstructure parameter separately while keeping the rest of the microstructure parameters fixed increases the work hardening of DP steel as shown in Figure 2.11.
Figure 2.11: The effect of each microstructure parameter on the flow stress (a) $d_m$, (b) $d_f$, (c) MVF, and (d) C wt%.

Thus, the 3D RVE model can predict any variation in the microstructure parameters. In order to calculate a tensile toughness as a response in the RSM model, the area under the flow curve for each design point was computed using the OriginLab software. Figure 2.12 shows a sample of the toughness measurement for design points (1), (10), and (22).

2.5.2 Analysis of RSM model

The statistical mathematical design basics, regression modeling approaches, and optimization processes are required to fit and find the appropriate response surface model from experimental data. The RSM usually includes all these methods.
Figure 2.12: Tensile toughness as measured under the predicted stress-strain curves for (a) DP#1, (b) DP#10, and (c) DP#22.

Thus, the RSM consists of a regression surface fitting to find the approximate responses and the design of experiments to determine minimum variances of the responses and optimizations utilizing the approximated responses. The RSM model was analyzed using MINITAB software after adding tensile toughness as the response in the designed analysis matrix as shown in Table 2.8. Additionally, the full quadratic model was chosen to investigate the RSM. The MRS results were presented in the form of 2D and 3D response surface charts. Statistical reports were also generated as detailed in Table 2.9, Table 2.10, and Figure 2.13.
Table 2.8: Microstructure parameters design matrix with results of tensile toughness

<table>
<thead>
<tr>
<th>Design Points (Run order)</th>
<th>Microstructure Parameters (Factors)</th>
<th>Response</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>d_r (µm)</td>
<td>d_m (µm)</td>
</tr>
<tr>
<td>DP#1</td>
<td>3.775</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#2</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#3</td>
<td>9.925</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#4</td>
<td>9.925</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#5</td>
<td>3.775</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#6</td>
<td>9.925</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#7</td>
<td>9.925</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#8</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#9</td>
<td>3.775</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#10</td>
<td>3.775</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#11</td>
<td>9.925</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#12</td>
<td>3.775</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#13</td>
<td>9.925</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#14</td>
<td>9.925</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#15</td>
<td>3.775</td>
<td>1.175</td>
</tr>
<tr>
<td>DP#16</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#17</td>
<td>3.775</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#18</td>
<td>9.925</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#19</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#20</td>
<td>3.775</td>
<td>0.725</td>
</tr>
<tr>
<td>DP#21</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#22</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#23</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#24</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#25</td>
<td>6.850</td>
<td>0.5</td>
</tr>
<tr>
<td>DP#26</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#27</td>
<td>6.850</td>
<td>1.4</td>
</tr>
<tr>
<td>DP#28</td>
<td>6.850</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#29</td>
<td>0.7</td>
<td>0.95</td>
</tr>
<tr>
<td>DP#30</td>
<td>13</td>
<td>0.95</td>
</tr>
</tbody>
</table>

Table 2.9 illustrates the analysis of variance that summarizes the statistical significance of each microstructure parameter on tensile toughness. Table 2.10 indicates RSM model regression evaluation (Analysis of Variance (ANOVA)) for tensile toughness. Figure 2.13 illustrates a matrix of interaction plots, which is the interaction of microstructure parameters on tensile toughness where demonstrates means for each range of a microstructure parameter with the range of a second microstructure parameter kept fixed.
Table 2.9: Analysis of Variance (ANOVA) results of the statistical significance of each microstructure parameters on tensile toughness (Estimated Regression Coefficients)

<table>
<thead>
<tr>
<th>Term</th>
<th>Coeff.</th>
<th>P-Value</th>
<th>VIF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant</td>
<td>+50.10</td>
<td>0.000</td>
<td>----</td>
</tr>
<tr>
<td>$d_m$</td>
<td>-6.59</td>
<td>0.000</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_m$</td>
<td>+89.10</td>
<td>0.864</td>
<td>1.00</td>
</tr>
<tr>
<td>MVF</td>
<td>+2.142</td>
<td>0.000</td>
<td>1.00</td>
</tr>
<tr>
<td>C wt%</td>
<td>+44.00</td>
<td>0.000</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_r$ * $d_f$</td>
<td>+0.326</td>
<td>0.028</td>
<td>1.05</td>
</tr>
<tr>
<td>$d_m$ * $d_m$</td>
<td>-48.50</td>
<td>0.071</td>
<td>1.05</td>
</tr>
<tr>
<td>MVF * MVF</td>
<td>-0.0395</td>
<td>0.002</td>
<td>1.05</td>
</tr>
<tr>
<td>C wt% * C wt%</td>
<td>-1054</td>
<td>0.042</td>
<td>1.05</td>
</tr>
<tr>
<td>$d_r$ * $d_m$</td>
<td>-0.020</td>
<td>0.995</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_r$ * MVF</td>
<td>+0.0274</td>
<td>0.584</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_r$ * C wt%</td>
<td>-0.0670</td>
<td>0.293</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_m$ * MVF</td>
<td>-0.0670</td>
<td>0.921</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_m$ * C wt%</td>
<td>+47.00</td>
<td>0.746</td>
<td>1.00</td>
</tr>
<tr>
<td>MVF * C wt%</td>
<td>+24.39</td>
<td>0.000</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Table 2.10: RSM model regression evaluation (Analysis of Variance (ANOVA) for tensile toughness)

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>Contribution</th>
<th>P-Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blocks</td>
<td>2</td>
<td>0.74%</td>
<td>0.041</td>
</tr>
<tr>
<td>Linear</td>
<td>4</td>
<td>88.85%</td>
<td>0.000</td>
</tr>
<tr>
<td>Square</td>
<td>4</td>
<td>2.74%</td>
<td>0.002</td>
</tr>
<tr>
<td>2-Way Interaction</td>
<td>6</td>
<td>6.51%</td>
<td>0.000</td>
</tr>
<tr>
<td>Lack-of-Fit</td>
<td>10</td>
<td>1.17%</td>
<td>0.132</td>
</tr>
<tr>
<td>Pure Error</td>
<td>3</td>
<td>0.00%</td>
<td>------</td>
</tr>
<tr>
<td>Total</td>
<td>29</td>
<td>100%</td>
<td>---</td>
</tr>
</tbody>
</table>

R-sq = 98.83%  
R-sq (adj) = 97.40%
As can be seen in Table 2.9, small p-values for ferrite grain size ($d_f$), martensite volume fraction (MVF), carbon content in DP steels (C wt%), ($d_f^2$), (MVF)$^2$, (C wt%)$^2$, and interaction of MVF and C wt% (p-values = 0.000, 0.042, and 0.028) indicate that these effects are statistically significant on the response. Slightly large p-values for martensite grain size ($d_m$), ($d_m^2$), interaction of $d_f$ and $d_m$, $d_f$ and MVF, $d_f$ and C wt%, $d_m$ and MVF, and $d_m$ and C wt% indicate that these effects are a certain trend toward quasi-significant. Variance inflation factors (VIF’s) that determine how much the variation of the predicted regression coefficients are exaggerated as corresponded to when the predictor variables are not linearly related are all close to 1. Thus, it indicates that the predictors are not correlated. VIF values greater than 5-10 suggest that the regression coefficients are poorly estimated due to severe multicollinearity. Therefore, the verified regression equation of toughness is as follows:
Toughness = 50.1 − 6.59(df) + 89.1(dm) + 2.142(MVF) + 44(C wt%) 
+ 0.326(df)^2 − 48.5(dm)^2 − 0.0395(MVF)^2 − 1054(C wt%)^2 
− 0.02(df × dm) 0.0274(df × MVF) − 11.3(df × C wt%) 
− 0.067(dm × MVF) + 47(dm × C wt%) + 24.39(MVF × C wt%)  

(2.14)

Table 2.10 outlines the linear terms, the squared terms, and the two way-interactions. The small p-values for the two way-interactions (p-value = 0.000), the linear terms (p-value = 0.002) and the squared terms (p-value = 0.000) imply there is curvature in the response surface. Furthermore, the contribution of these terms confirms the existence of the curvature of the response surface. Significantly, this curvature is usually present when parameters settings are near a maximum or minimum response value. Moreover, the p-value for lack of fit is 0.132 signifying that this model appropriately fits the data. The R^2 indicates that the predictors describe 98.83% of the variance in toughness. The adjusted R^2 is 97.40%, which estimates the number of predictors in the model. Both estimations show that the model fits the data well.

Figure 2.13 presents interaction plots to visualize possible interactions when the influence of one factor relies on the level of the other factors, which are beneficial for estimating the presence of interaction. Parallel lines in Figure 2.13 mean there is no any interaction between parameters. Nonetheless, any notable difference in tendency between lines indicates the significant level of interaction, in the last two columns, there are no parallel lines indicating that the influence of MVF and C wt% upon toughness depend upon df and dm as shown in Figure 2.13. The interaction between MVF and df takes place when the change in toughness from a low level to a high level of MVF (14.23% to 36.075%) is not the same as the change in toughness at the same two levels of df (3.78 to 9.93 μm); the interaction between C wt% and df has the same effect. Another key thing to
remember is that these plots can be used to compare the main influences and interaction influences, provided that evaluating significance is determined by looking at the p-values for all interaction effects in the Analysis of Variance and RSM model regression evaluation as shown in Table 2.9 and Table 2.10.

The effects of microstructure parameters on toughness are presented in Figure 2.14 to Figure 2.19 as contours and three-dimensional graphs that were obtained using MINITAB software. All these graphs are held and identified at middle values of microstructure parameters.

![Figure 2.14: 3D surface and contour plot for toughness with ferrite grain size (df) and martensite grain size (dm)](image)

As it is shown in Figure 2.14, the 3D surface presents the three-dimensional relationship of toughness with ferrite grain size (df) and martensite grain size (dm) with the parameters on the x and y-axis and the fitted response on the z-axis represented by a smooth surface. As shown in this plot, for fixed df, the toughness increases with increasing dm up to about 1.00 μm then it drops. The df becomes strongly significant at about 3 μm (and below) at which the toughness increases dramatically with decreasing df. Unlike dm, the effect of df on toughness follows the Hall-Petch
relation of strength versus grain size. Furthermore, the contour plot presents the three-dimensional relationship of toughness with ferrite grain size ($d_f$) and martensite grain size ($d_m$) in two dimensions (2D) where the x and y-axis are parameters, and contours represent the fitted response. The darker regions indicate higher toughness where the contour levels reveal a peak at the middle left of the plot, which is greater than 180 MJ/m$^3$. Moreover, the contour plot shows that toughness increases as $d_f$ decrease at the middle values of $d_m$. To put it another way, the plot shows that increasing in toughness from the lower range to the higher range $d_f$ is greater at the middle range of $d_m$. 

**Figure 2.15**: 3D surface and contour plot for toughness with ferrite grain size ($d_f$) and martensite volume fraction (MVF)

The 3D surface plot in Figure 2.15 demonstrates that the rise in toughness from the low to the high level of MVF is larger at the lower values of $d_f$. Another key point to remember in Figure 2.15 is that the 2D contour plot indicates that the largest toughness is achieved when $d_f$ values are low, and MVF values are high. This highest toughness range shows at the upper left corner of the plot, which is greater than 220 MJ/m$^3$. 

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In Figure 2.16, the 3D surface plot shows that toughness increases as the C wt% increases and the $d_f$ declines. In the contour plot, because there are 3 contours across the top of the plot and 2 contours across the bottom of the plot, the plot shows that the growth in toughness from the lower to the higher value of C wt% is larger at the high values of $d_f$. Similar to Figure 2.15, the higher toughness values that are greater than 200 MJ/m$^3$ are located in the upper left of the contour plot.

As can be seen in the 3D surface plot in Figure 2.17, the toughness rises sharply as C wt% increases; conversely, the toughness climbs slowly as the $d_m$ increases up to about 1.00 μm, then it declines. Moreover, the contour plot in Figure 2.17 reveals that maximum toughness is obtained when C wt% values are high, and $d_m$ levels are at middle values. This maximum toughness region that is greater than 180 MJ/m3 shows in the upper middle of the plot.

By examining the 3D surface plot in Figure 2.18, there can be seen a steadiness in the toughness with increasing $d_m$; on the other hand, there is an upward trend in the toughness with rising C wt% values. In the contour plot, because there are 4 contours across the left of the plot
and 1 contour across the bottom of the plot, the plot presents that the C wt% has a significant effect
on toughness while the d_m has little to no effect on toughness. Regarding the interaction plots in
Figure 2.13, there are no parallel lines for the interactions between d_m and C wt%. The p-value for
these interactions is also high (p-value = 0.746).

Figure 2.17: 3D surface and contour plot for toughness with martensite grain size (d_m) and
carbon content in DP steel (C wt %)

Figure 2.18: 3D surface and contour plot for toughness with martensite grain size (d_m) and
martensite volume fraction (MVF)
As follows from Figure 2.19, shown above, the 3D surface plot indicates that toughness upsurges as both MVF and C wt% increase. The contour chart also demonstrates that the growth in toughness from the lower to the higher value of MVF is larger at the high values of C wt%; thus, the maximum toughness is located at the top right of the contour plot.

All things considered, the increase in MVF can indirectly affect the response – toughness – in two methods. Firstly, the increase in the martensitic transformations creates more quantities of geometrically necessary dislocations (GNDs). Thus, the GNDs are essentially formed at the grain boundaries between ferrite and martensite phase and strengthen the ferrite phase. Secondly, a rise in the amount and the grain size of the martensite islands with increasing MVF induces a reduction in the $d_f$. By growing the hardening of the ferrite phase, these two influences, in turn, improve the strength of DP steel as in Ref [79]. Another key thing to remember, in this paper, the only back stress that is considered results from incompatibilities between martensite phase as a hard phase and ferrite phase as soft matrix, which is dealt within the homogenization model. Moreover, many preexisting research methodologies studied individually one class of DP steel.
where C wt% and MVF were not effectively connected. By contrast, the present study allows us to assess the impact of the amount of the martensite phase (MVF) in direct connection to its carbon content as in Eq (2.5). Consequently, it can be seen from the results that for the toughness of DP steel with low C wt%, the MVF has a higher effect on the toughness, due to the decreasing carbon content of the martensite with the increase in MVF. The opposite occurs for toughness with high C wt%. It is observed in this study that a rise in the carbon content (C wt%) significantly affects the properties of DP steel, inducing an improvement in the toughness of DP steel. That is to say, the GNDs at the ferrite–martensite interfaces that are formed by changing austenite phase to the martensite phase goes up with rising C wt%. The results show that due to the GND’s effect, the higher MVF and smaller \( d_f \) has a significant influence in the toughness of DP steels. The strength and ductility combination in DP steel were strongly affected by MVF, C wt%, and \( d_f \). Importantly, the higher values of toughness are obtained at an intermediate \( d_m \) by changing the other microstructure parameters, which can be considered as the optimum \( d_m \). Size effect of the ferrite phase obviously complies with the Halle-Petch relation; on the other hand, the effect of martensite grain size does not obey it.

The optimization chart, Figure 2.20, presents the influence of each microstructure parameter (columns) on the responses, toughness of DP steel. The perpendicular red lines on the plot illustrate the existing parameter arrangement and the values in red shown at the top of a column exhibit the existing parameter value settings. The black dashed line and blue values describe the responses for the existing parameter values.
The desirability (D=0.7656), as shown in Figure 2.20, shows how well a combination of microstructure parameters satisfies a toughness optimum and are more effective at maximizing toughness. As shown in Figure 2.20, an optimum ferrite grain size \( (d_f) \) is 0.7 μm, optimum martensite grain size \( (d_m) \) is 0.99 μm, optimum martensite volume fraction (MFV) is 47%, and optimum carbon content in DP steel is 0.230 wt% which resulted in toughness of 324.23 MJ/m\(^3\). The optimal solution can be modified by altering the settings to see how different settings affect responses interactively. As previously mentioned, the maximum toughness was obtained at an intermediate \( d_m \) as shown in the second column in Figure 2.20. Comparing these results with literature finding, the 47% optimum MFV and 0.230 wt% optimum C wt% is in agreement with Ref’s [67,76].

2.6 Conclusions

The 3D RVE modeling of flow stress of DP steels were conducted using the 3D representative volume element (3D RVE) and the response surface method (RSM) by statistically and independently varying four microstructure parameters: the ferrite grain size \( (d_f) \), the martensite grain size \( (d_m) \), the martensite volume fraction (MVF), and the carbon content in DP steel (C wt%).
The response surface methodology (RSM) was employed to determine the required points of analysis within concerned ranges of these microscopic parameters, which proves to be a powerful tool for studying these parameter effects on a combination of strength and ductility, and also to find the optimum microstructure parameters. This study clearly shows that:

1) Not only numerical prediction from the 3D RVE model was in good agreement with the flow curve of DP500 (with a less than 4% error), but also the model contributes further understanding into improving strength and ductility combination of DP steels.

2) The parametric study based on the influence of variations of microscopic parameters revealed that the microstructure parameters play an important role in the mechanical behavior of DP steels. It was shown that for these microscopic parameters, the energy absorption capacity of material would be optimized.

3) It has been demonstrated through the parametric study that the ferrite grain size ($d_f$), the martensite volume fraction (MVF), the carbon content in DP steel (C wt%), and their interactions were statistically significant with regards to the combination of strength and ductility of DP steel. Having said that, the martensite grain size and its interaction showed a certain trend toward quasi-significant. Furthermore, it was found that the full quadratic equation that describes the relationship between the microscopic parameters and the response fitted the data well based on the $R^2$ (98.83%) and the adjusted $R^2$ (97.40%).

4) The energy absorption of DP steels was strongly affected by the martensite volume fraction (MVF), the carbon content (C wt%), and its interactions, and by increasing both of them the energy increases. However, the low values of the ferrite grain size ($d_f$) (below 4 μm) had a significant effect on toughness, which makes the increase drastic with decreasing $d_f$. An
important point made through these findings is that the greater values of energy absorption of DP steels were achieved at a mean ($d_m$), which was recognized as the optimum $d_m$.

5) The RSM optimization predicts that an optimum energy absorption of DP steels is $\approx 324$ and this can be achieved at a $0.7 \, \mu m$ ferrite grain size ($d_f$), $1 \, \mu m$ martensite grain size ($d_m$), 47% martensite volume fraction (MVF), and 0.23 wt% carbon content in DP steel ($C \, \text{wt}\%$).

6) Finally, the findings from this study suggest that the automobile designers need to match the component requirements to the energy absorption for DP steels can be achieved by modifying the setting of microscopic parameters interactively to produce a material suitable for the intended application. Therefore, the desirable microstructure parameters of DP steels can be controlled by varying intercritical heat treatment temperatures as in Ref [23].

Acknowledgments

The author would like to acknowledge the Libyan Ministry of Higher Education and Scientific Research and Mrs. Cassandra Radigan, Educational Program Manager at MSC Software.
Recent studies on developing dual phase (DP) steels showed that the combination of strength/ductility could be significantly improved when changing the volume fraction and grain size of phases in the microstructure depending on microstructure properties. Consequently, DP steel manufacturers are interested in predicting microstructure properties as well as optimizing microstructure design at different strain rate conditions. In this work, a microstructure-based approach using a multiscale material and structure model was developed. The approach examined the mechanical behavior of DP steels using virtual tensile tests with a full micro-macro multiscale material model to identify specific mechanical properties. Microstructures with varied ferrite grain sizes, martensite volume fractions, and carbon content in DP steels were also studied. The influence of these microscopic parameters at different strain rates on the mechanical properties of DP steels was examined numerically using a full micro-macro multiscale finite element method. An elasto-viscoplastic constitutive model and a response surface methodology (RSM) was used to determine the optimum microstructure parameters for a required combination of strength/ductility at different strain rates. The results from the numerical simulations are compared with experimental results found in the literature. The developed methodology proved to be a powerful tool for studying the effect and interaction of key strain rate sensitivity and microstructure parameters on mechanical behavior and thus can be used to identify optimum microstructural conditions at different strain rates.
3.1 Introduction

An effective approach to decrease vehicle body is to utilize thinner sheet steels while maintaining safety criteria. This approach requires developing materials with a good combination of strength and ductility to meet crashworthiness and metal forming processes criteria. Even though one may consider a number of possibilities of lightweight materials with desirable strength, the material formability adds to the practical limits of its forming process. Nonetheless, materials for automotive applications should meet specific criteria that are required to pass collision-related tests before forming materials into different vehicle components [80]. Recently, automobile manufacturers have employed dual phase steel (DP) grades due to its good combination of both strength and formability [81]. DP steels have been successfully utilized in automobile components that need crashworthiness resistance for its good advantage in decreasing car weight with enhancing safety criterions, along with their benefits of reduced manufacturing cost through the use of cold forming processes instead of the hot forming processes.

The microstructure of DP steels includes martensite phase particles dispersed in the soft ferritic matrix. Generally, DP steels contain a purely ferrite phase as a matrix with about a 3.3–47% fraction of martensite islands spread as a hard phase over a matrix [48]. Several studies examined the influence of strain rate on the plastic behavior of DP steels under both quasi-static and dynamic loading conditions; examples include these references [1,2,24,32,50,66,80–95]. However, only a limited number of investigations have examined the influence of the microstructure parameters and the role they play in affecting the plastic behavior of DP steels under quasi-static and dynamic loading conditions [80,87,89]. For example, Alturk et al. [80] investigated the influence of martensite phase content in DP980 and QP980 on the strain rate sensitivity at different strain rates 0.005 and 500 sec\(^{-1}\); Kim and Lee [87] studied the influence of
tempering and martensite morphology on plastic behavior of DP steels under quasi-static and
dynamic loading; and Hwang et al. [89] investigated the influence of microscopic parameters such
as martensite volume fraction and ferrite grain size on dynamic torsional behavior and quasi-static
tensile in DP steels. Other investigations attempted to enhance the plastic behavior of DP steels
under both quasi-static and dynamic loading conditions by acquiring effective methods to verify
the optimum microscopic parameters and obtain a maximum strength–ductility combination and
identification of the effective microstructure parameters[2,32,66,94,95]. For example, Delincé et
al. [66] developed a simple physical model for the work hardening behavior of DP steels and
performed statistical investigation on the effect of martensite volume fraction, ferrite grain size,
and carbon content on the flow stress of DP steels under quasi-static loading condition.
Nevertheless, although these works and others have extensively studied DP steels both
computationally and experimentally, there is a need for a comprehensive statistical study of the
effect of basic microscopic feature and the role they play in influencing the strain rate sensitivity
of DP steels. To that end, in this work a multiscale material modeling approach of DP steels is
utilized along with a statistical and mathematical tool to create an efficient analytical methodology
for verifying the optimum microstructure parameters under quasi-static and dynamic loading
conditions.

The multiscale approach developed in this work uses a mean-field homogenization
incremental formulation to predict the nonlinear mechanical behavior of DP steels and examine
the influences of microstructure parameters namely: ferrite grain size ($d_f$), martensite volume
fraction ($V_m$), and Carbon content (C wt%) on the flow stress of DP steels under different strain
rates ($\dot{\varepsilon}$). Martensite grain size is assumed to be 1 μm based on the preliminary trials and
preexisting literature, which points out that the martensite grain size does not have a significant
effect on yield stress and ultimate strength of DP steels [82]. The “Digimat” software and its interface to structural FEA software facilitate multiscale finite element analysis of DP steel microstructure under different strain rates. The multiscale structural modeling tool (Digimat-CAE) (i.e. The Linear and nonlinear multiscale material modeling software from e-Xstream engineering) that sets the interface between the mean-field homogenization incremental formulation (Digimat-MF) and structural analysis software (LS-DYNA) is used to accurately predict the flow behavior of DP steels in uniaxial tension under quasi-static and dynamic loading. The simulation is then utilized to perform a parametric study on the effect of various microstructure parameters on plastic behavior under quasi-static and dynamic conditions. Specifically, the current study investigates the effect of microstructure parameters ($d_i, V_m, C$ wt%, and $\dot{\varepsilon}$) in DP steels on the combination of strength and ductility. A dislocation density based nonlinear elastic-viscoplastic model that can predict the flow stress of DP steels under quasi-static and dynamic uniaxial loading conditions is developed, and the model is then used to generate a parametric study on the influence of microscopic parameters on the inelastic behavior. This is followed by a systematic response surface methodology (RSM) investigation of the effect of microstructure factors 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 at different strain rate conditions.

3.2 Multiscale Material Modeling

Not only a multiscale material computational modeling was a necessity for studying the effect of microstructure parameters, but also it is essential for directing the material design of DP steels to enhance its strength and ductility. For that reason, the mean-field homogenization incremental formulation (Digimat-MF) that aims at predicting the flow stress of DP steels based
on the constitutive equation of ferrite and martensite phase is used to link structural FEA software (LS-DYNA) through LS-DYNA user-defined material (UMAT) code. This model enables upstream and downstream two-scale material modeling. LS-DYNA is carried out at the macro-scale, and for each time interval \( (t_n, t_{n+1}) \) at each integration point (IP) of the macro FE mesh, LS-DYNA/UMAT calls Digimat-MF through Digimat-CAE to perform the homogenization scheme of two phases (ferrite and martensite). The macro strain \( (\varepsilon) \), materials constant, and history variables at \( t_n \) are passed by UMAT to Digimat-MF to compute the macro stress \( (\sigma) \) and macro tangent moduli \( (C) \) at \( t_{n+1} \). The micro-structure of two phases are not “seen” by LS-DYNA but only by Digimat-MF, which takes into account each integration point to be the center of a representative volume element (RVE) which contains the heterogeneous micro-structure of two phases as shown in Figure 3.1.

### 3.2.1 Constitutive equations description and parameter identification

In this study, a dislocation density constitutive formulation \([2,25,26,51,64,70,73–75,96]\) is used for ferrite and martensite phase. In this formulation, the dependence of the flow stress on dislocation density is given by the following relation.

\[
\sigma_{\text{flow}}^{f,m} = \sigma_{y0}^{f,m} + \langle \alpha M \mu b \sqrt{\rho} \rangle \wedge (f, m). \text{f and m refer to ferrite and martensite phase}\quad (3.1)
\]

where \( \alpha \) is a constant, \( M \) is the Taylor factor, \( \mu \) is the shear modulus, \( b \) is the Burger’s vector, and \( \rho \) is the dislocation density. The first term in Eq (3.1) is the initial yield stress that is independent of dislocation density and consists of the following hardening components:

\[
\langle \sigma_y \rangle \wedge (f, m) = \sigma_g \wedge (f, m) + \Delta \sigma_{c}^{f,m} + \sigma_S \quad (3.2)
\]
Figure 3.1: Multiscale material modeling using Digimat as the material modeler and LS-DYNA as structural FEA software
where $\sigma_g$ is grain size effect, $\Delta \sigma_c$ is precipitation hardening, and $\sigma_s$ is solid solution hardening. The grain size effect is expressed by Hall-Petch model:

$$\sigma_f^m = \frac{K_{HP}}{\sqrt{d_f^m}}$$ (3.3)

Here, $K_{HP}$ is Hall-Petch constant and $d_f$ or $m$ is grain size of ferrite or martensite phase. The second term in Eq (3.2) represents precipitation hardening based on carbon content in solid solution. In the case of ferrite, it is given by the following relation [2,51,70,97].

$$\Delta \sigma_c^f = 5000 \times \%C_{ss}^f$$ (3.4)

In the case of martensite, the relationship between the martensite precipitation hardening and the carbon content in martensite phase is a linear relationship, which is in agreement with experimental results obtained in [66,98,99], and is given by the following equation.

$$\Delta \sigma_c^m = \sigma_{y0}^m|_{\%C_{ss}^m=0} + Cs \times \%C_{ss}^m$$ (3.5)

where $\sigma_{y0}^m|_{\%C_{ss}^m=0}$ is the initial yield stress of martensite at zero carbon content, which is the extrapolated from experimental results in [98] at carbon free. $Cs$ is the carbon sensitivity and $\%C_{ss}^f$ and $\%C_{ss}^m$ is wt.% carbon content in solid solution in ferrite and martensite, respectively. The carbon content in the ferrite phase is assumed to be 0.02%, which is the solubility limit for carbon in ferrite at room temperature. Even though the increase in the flow and tensile strengths with increasing martensite volume fraction at a defined carbon content in the martensite phase is noted and broadly reported (e.g. [100–102], to cite only a few), the law of mixture can be used to
calculate the carbon content in the martensite phase based on the carbon content in DP steel [70].

It can be described as:

\[
\%C_{ss}^{DP} = \%C_{ss}^f \times V_f + \%C_{ss}^m \times V_m
\]  

where \( \%C_{ss}^{DP} \) is the nominal carbon composition of the DP steel, and \( V_f \) and \( V_m \) are the ferrite volume fraction and martensite volume fraction, respectively. Although this may be considered as a simplification, it is considered as a reasonably suitable approximation. The last term in Eq (3.2) is the contribution of the solid solution hardening and the effects of alloying elements in solid solution and it can be described as [2,51,64,70]:

\[
\sigma_0 (\text{in MPa}) = 77 + 80\%\text{Mn} + 750\%\text{P} + 60\%\text{Si} + 80\%\text{Cu} + 45\%\text{Ni} \\
+ 60\%\text{Cr} + 11\%\text{Mo} + 5000\%\text{N}
\]  

(3.7)

In this model, the solid solution stress is calculated at the middle of the alloying elements ranges in DP steels, which is 274 MPa.

According to the Mecking-Kocks theory, the rate of dislocation density evolution to shear strain during the deformation is the result of the competition between the rate of production of dislocation and the annihilation rate of dislocation [2], which can be written as:

\[
\frac{d\rho}{d\gamma} = \frac{d\rho}{d\gamma}_{\text{stored}} + \frac{d\rho}{d\gamma}_{\text{recovery}} = \frac{1}{bL} - k_r \rho
\]  

(3.8)
where $L$ is the dislocation mean free path and $k_r$ is a constant. Rodriguez and Gutierrez [103] further developed this concept for the ferritic and martensitic phase; thus, the effective stress-strain relation is given by:

$$
\Delta \sigma = \alpha M \mu \sqrt{b} \left(1 - \exp\left(-\frac{M k_r \varepsilon}{k_r L}\right)\right)
$$

(3.9)

Once the description of the three terms in Eq (3.1) has been defined, the complete methodology for defining the flow stress of each phase in the DP steel is:

$$
\sigma_{flow}^{f,m} = \sigma_{0}^{f,m} + \alpha M \mu \sqrt{b} \left(1 - \exp\left(-\frac{M k_r \varepsilon}{k_r L}\right)\right)
$$

(3.10)

where $\sigma_{flow}$ and $\varepsilon$ are responsible for the true flow stress (von Mises stress) and true strain, respectively.

In order to conduct a finite element analysis of the low and high strain rates tensile experiments on the multiphase material, a more convenient constitutive equation of each phase is required, which describes the hardening behavior in terms for strain (as opposed to dislocation density) as measured in the experiments. Consequently, it is important to take into account an elasto-viscoplastic (EVP) constitutive model such as Current yield Norton law, which is frequently utilized to describe the flow stress of multiphase materials at different strain rates [22]. In this study, the current yield Norton model was employed in the Digimat-MF model for modeling ferrite phase in the DP steels. This ferrite phase model includes von Mises plasticity model, with assuming isothermal conditions and neglecting temperature increase due to plastic dissipation,
associated flow rule, combined power law isotropic hardening, and strain-rate effects. In this model, after stress exceeds the initial yield stress ($\sigma_{y0}$), the Cauchy stress is given by:

$$\sigma_{eq}^f = \sigma_{y0}^f + K^f \varepsilon_p^{nf}$$  \hspace{1cm} (3.11)

with

$$\sigma_{eq}^f = \sqrt{\left(\frac{2}{3} S^f : S^f \right)}, \quad S^f = \sigma^f - \frac{1}{3} \sigma_{kk}^f I$$  \hspace{1cm} (3.12)

On the other hand, the exponential law was used to describe flow stress of martensite phase, which is recommended by Digimat for material exhibits a horizontal plateau in the stress-strain curve, and was used successfully by Pierman et al. [104] to fit experimental data of bulk martensite samples. The following equation is expressed the Cauchy stress:

$$\sigma_{eq}^m = \sigma_{y0}^m + R\left[1 - \exp(m\varepsilon_p)\right]$$  \hspace{1cm} (3.13)

The evolution of the viscoplastic flow rule obeys the following flow rule:

$$D^{vpf} = \frac{3}{2} \frac{\dot{\varepsilon}_{vp}^f}{\sigma_{eq}^f} S^f$$  \hspace{1cm} (3.14)

$$\dot{\varepsilon}_{vp}^f = \frac{\sigma_{y0}^f}{\beta} \left[\frac{\sigma_{eq}^f - \sigma_{y0}^f - K^f \varepsilon_p^{nf}}{\sigma_{eq}^f}\right]^{m^*}$$  \hspace{1cm} (3.15)
Here, $\beta$ (1000 MPa. sec) is the viscoplastic coefficient, which expresses the viscoplastic sensitivity of the multiphase materials to the strain rate, and $m^*$ (1) is the viscoplastic exponent of the current yield Norton according to [22]. $K^f$, $n^f$, $R$ and $m$ are the ferrite hardening modulus, the ferrite strain hardening exponent, the martensite hardening modulus and the martensite strain hardening exponent respectively, which are obtained by curve fitting equations (3.11) and (3.13) to the data obtained from Eq (3.10). Another key thing to mention, at high strain rates, is that the material temperature increases due to conversion of plastic work to heat. Tarigopula et al. [105] calculated experimentally the rise in temperature at the high strain rate for DP800, and they found that the temperature was gradually changed from room temperature to approximately 60K in the region of large strain at a strain rate of 445 sec$^{-1}$, which is neglected and considered a moderate temperature rise. In this study, an increase in temperature is assumed to be negligible and the isothermal condition in this model is considered. The parameter values that are used for the ferrite and martensite phases in multiscale material model simulation are listed in Table 3.1.

### 3.2.2 Homogenization technique

A mean-field homogenization (MFH) model was used to calculate the volume average of stress and strain states at the macro scale (RVE) and microscale (each phase) [106]. In the multiscale material model, the macro strain is known at each macroscopic point $\bar{x}$, which is the center of RVE of the multiphase material, DP steel. At the microscale level, $\omega$ is the domain of RVE and $\delta_\omega$ is the RVE boundary. Three steps describe the homogenization scheme in general as shown in Figure 3.2.
Table 3.1: Description of the different materials parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Magnitude (Unit)</th>
<th>Used in Eq.</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Taylor constant</td>
<td>$\alpha$</td>
<td>0.33</td>
<td>(1), (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Taylor factor</td>
<td>$M$</td>
<td>3</td>
<td>(1), (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Shear modulus</td>
<td>$\mu$</td>
<td>80000 (MPa)</td>
<td>(1), (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Magnitude of the Burgers vector</td>
<td>$b$</td>
<td>$2.5 \times 10^{-10}$ (m)</td>
<td>(1), (8) (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Hall–Petch constant</td>
<td>$K_{HP}$</td>
<td>150 (MPa$\sqrt{mm}$)</td>
<td>(3)</td>
<td>[66]</td>
</tr>
<tr>
<td>Carbon content in ferrite</td>
<td>$%C_{ss}$</td>
<td>0.02 (wt %)</td>
<td>(4)</td>
<td>[100,101]</td>
</tr>
<tr>
<td>Initial yield stress of martensite phase</td>
<td>$\sigma_{m}^0$</td>
<td>1250 (MPa)</td>
<td>(5)</td>
<td>[66]</td>
</tr>
<tr>
<td>Carbon sensitivity constant</td>
<td>$Cs$</td>
<td>1600 (MPa/wt %)</td>
<td>(5)</td>
<td>[66]</td>
</tr>
<tr>
<td>Peierls stress</td>
<td>$\sigma_0$</td>
<td>274 (MPa)</td>
<td>(7)</td>
<td>---</td>
</tr>
<tr>
<td>Dislocation mean free path in ferrite</td>
<td>$d_f$ (µm)</td>
<td>(8), (9), (10)</td>
<td>[2,51,70,77]</td>
<td></td>
</tr>
<tr>
<td>Dislocation mean free path in martensite</td>
<td>$L$</td>
<td>$3.8 \times 10^{-8}$ (m)</td>
<td>(8), (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Recovery rate in ferrite</td>
<td>$k_r$</td>
<td>$10^5 / d_f$</td>
<td>(8), (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Recovery rate in martensite</td>
<td>$k_r$</td>
<td>41</td>
<td>(8), (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
</tbody>
</table>
Figure 3.2: Multiscale model scheme

The centralization step is the first step, where the given macroscopic strain is centralized in each phase (ferrite and martensite phase). The second step is microscopic calculation of stress for each phase based on the defined constitutive equations. In the third step, a specific homogenization technique is applied to average the microscopic stress field and to obtain a macroscopic stress field. Thus, the multiscale model of multiphase materials relies explicitly on the behavior of the microstructure constituents, the current shape of inclusion and its orientation. For the case of DP steels, the ferrite phase and martensite phase extend on domain $\omega_f$ and $\omega_m$ respectively and each phase has volume $v_f$, $v_m$ respectively. Then the ferrite volume fraction can be expressed by [38]:

$$\text{volume fraction} = \frac{v_f}{v_f + v_m}$$
\[ V_f = \frac{V_r}{V}, \text{ where } V \text{ is the RVE volume} \quad (3.16) \]

and for martensite phase:

\[ V_m = \frac{V_m}{V} = 1 - V_f \quad (3.17) \]

The volume average of the RVE and each phase can be written as:

\[ \bar{\nu} = \frac{1}{V} \int_{\omega_f} f(x, \bar{x}) d\nu \ldots \ldots \text{ for the RVE} \quad (3.18) \]

\[ \bar{\nu}_{f,m} = \frac{1}{V_{f,m}} \int_{\omega_{f,m}} f(x, \bar{x}) d\nu_{f,m} \ldots \ldots \text{ for each phase} \quad (3.19) \]

Then the total volume of the RVE is the sum of the two:

\[ \bar{\nu} = V_f (\bar{\nu}_f)_{\omega_f} + V_m (\bar{\nu}_m)_{\omega_m} \quad (3.20) \]

And thus, the volume average of strain field over the RVE is given by:

\[ \bar{\epsilon}_\omega = V_f (\bar{\epsilon}_f)_{\omega_f} + V_m (\bar{\epsilon}_m)_{\omega_m} \quad (3.21) \]

Equation (3.16) can be applied on any micro field variable such as stress field. The relation between the strain volume average overall inclusions (martensite islands) and the strain volume average over the matrix (ferrite phase) is expressed in any MFH model by the so-called strain concentration tensor \( (B^{\epsilon}) \) and for the micro strain (the strain volume average over the RVE) via \( (A^{\epsilon}) \) as follows [106]:
\[(\bar{\varepsilon}_m)_{\omega_m} = B^e: (\bar{\varepsilon}_f)_{\omega_f}\]  
\[(\bar{\varepsilon}_f)_{\omega_f} = A^e: \bar{\varepsilon}_\omega\]  

(3.22)  
(3.23)  

\(B^e\) and \(A^e\) are not independent, and \(A^e\) can be calculated from \(B^e\):

\[A^e = B^e: [V_m B^e + (1 - V_m)I]^{-1}\]  

(3.24)  

These calculations are applicable for any multiphase material model.

Homogenization schemes are fundamentally based on the Eshelby’s solution except for the simplest schemes such as Voigt and Reuss schemes wherein Voigt scheme, a uniform strain over the RVE is supposed, and in Seuss scheme, a uniform stress is assumed [38,107]. Based on the Eshelby’s solution, the strain field in the single ellipsoidal inclusion is uniform and related to the remote macro strain as follows:

\[\bar{\varepsilon}_m (x) = H^e (I, C_f, C_m): \bar{\varepsilon} \quad \forall x \in (I)\]  

(3.25)  

where \(H^e, C_f, C_m\) are the single inclusion strain concentration tensor, the ferrite uniform stiffness, and the martensite uniform stiffness, respectively.

with,

\[H^e (I, C_f, C_m) = [I + \xi (I, C_f): C_f^{-1}: (C_m - C_f)]^{-1}\]  

(3.26)
Where $\xi(I, C_f)$ is Eshelby’s tensor which is a function of the isotropic elastic properties of ferrite and the shape of the martensite phase. For multiphase materials including only two phases such as DP steels, a Mori-Tanaka model has been proposed by Tanaka and Mori [71]. In this model, they supposed that the inclusions in the RVE undergo the matrix strain as the far-field strain in the Eshelby’s solution as follows:

$$
(\bar{\varepsilon}_m)_{\omega_m} = \left[ I + \xi(I, C_f) : C_f^{-1} : (C_m - C_f) \right]^{-1} : (\bar{\varepsilon}_f)_{\omega_f}
$$

$$
B^\varepsilon = H^\varepsilon (I, C_f, C_m)
$$

This leads us to that the Mori-Tanaka model is attractive for multiphase materials like DP steels. In addition, it has a physical explanation, which makes each inclusion acts in the same way as an isolated inclusion in the matrix seeing $(\bar{\varepsilon}_f)_{\omega_f}$ as a far strain field [38,71,106,107].

### 3.3 Response Surface Methodology (RSM)

RSM is employed to examine the relationship between a response variable and a set of factors [78,108]. In this study, RSM was utilized to define the required analysis points (the simulation settings) within specified ranges of microstructure parameters and strain rate ($\dot{\varepsilon}$): a $d_f$ range of 0.7 – 13 µm, a $V_m$ range of 3.3 – 47%, and a C wt% ranges 0.06 – 0.15 wt % in DP steels and a $\dot{\varepsilon}$ ranges of 0.005-500 sec$^{-1}$. The ranges of microstructure parameters ($d_f$, $V_m$, and C wt%) were estimated based on the previous literature review and a few preliminary trials. In addition, strain rate ($\dot{\varepsilon}$) range were chosen according to their lifetime of automotive materials [80]. The multiscale material modeling was conducted according to the simulation points in the design
matrix obtained from RSM. This RSM model initially allowed us to design the experiment effectively, and then provided data for a parametric study and optimization.

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. The complete quadratic polynomial regression model as shown in Eq (3.28) was determined for predicting the response variable \( F \) in terms of the independent variables \( (X_1, X_2, X_3, X_4) \), that are the microstructure parameters and strain rate. The RSM model is a straightforward power series expansion of the following form.

\[
F = a_0 + a_1X_1 + a_2X_2 + a_3X_3 + a_4X_4 + a_{11}X_1^2 + a_{22}X_2^2 + a_{33}X_3^2 + a_{12}X_1X_2 + a_{13}X_1X_3 + a_{14}X_1X_4 + a_{23}X_2X_3 + a_{24}X_2X_4 + a_{34}X_3X_4
\]  

(3.28)

Thereafter, the multiscale material model of DP steels was performed for the ultimate strength \( \sigma_u \) and ductility \( \varepsilon_u \% \) then introduced into the previously designed matrix.

To evaluate the metal forming performance, maximum ultimate strength, and a satisfactory formability would be a good measurement for the light, strong DP steels. When the RSM model is introduced, the results are presented in the form of 3D and 2D diagrams. These charts exhibit how the response variable is a function of four factors based on a model regression as shown in Eq (3.28).

3.4 Simulation Procedure

In this study, 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...
The micro-macro multiscale material model of the flow behavior of DP steels was implemented in six steps: (1) An analysis matrix that contains design points was designed and created using Minitab as mentioned in section 3.3. (2) An appropriate flow behavior of the ferrite and martensite phases were determined according to Eq (3.10) and the required parameters that are listed in Table 3.2. (3) The OriginLab software was conducted to fit an elasto-viscoplastic (EVP) constitutive model to the analytical flow stress of ferrite and martensite phase (Eq (3.10)) to define mechanical constants of constituents for all design points. (4) Flow curves of two phases for each design point were introduced to Digimat-MF. (4) Coupling Digimat-MF to LS-DYNA via UMAT/Digimat-CAE was performed, and loading and boundary conditions were defined in LS-DYNA (5) The flow curve of the micro-macro multiscale material model for each design point in coupling Digimat-MF to LS-DYNA was obtained. (6) An analysis of the RSM model by adding ultimate strength and ductility for each design point to the design of the analysis matrix was carried out to obtain 2D contour plots, 3D surface plots, and the microstructure parameters optimization. Thus, the OriginLab software was performed to fit equation (3.11) and (3.13) to the analytical flow stress of ferrite and martensite phase to define mechanical constants of constituents for all design points. What follows in Table 3.2 and Figure 3.3 is an example of these implementations of the Curve Fitting application in OriginLab software for design points (2) to determine the fitting constants of the constituents for all design points.

The simulated tension tests under both quasi-static and dynamic strain rate conditions were performed to determine the flow stress for each design point. Specimen dimensions that were used in the simulation were identical to those that were used in the experimental tests.
Table 3.2: The analytical and fitted flow stress of DP steel constituents for design points (2)

<table>
<thead>
<tr>
<th>Flow stress according to Eq. (3.10)</th>
<th>Flow stress according to fitted Eq. (3.11) and (3.13)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{flow} = 332 + 1.25 \times \sqrt{(1 - \exp(-4.38\varepsilon_p)/(10^{-5}))}$</td>
<td>$\sigma_{flow} = 332 + 659\varepsilon_p^{0.451}$</td>
</tr>
<tr>
<td>$\sigma_{flow}^m = 1978 + 1.25 \times \sqrt{(1 - \exp(-123\varepsilon_p)/(1.56 \times 10^{-5}))}$</td>
<td>$\sigma_{flow} = 1978 + 975[1 - \exp(-309\varepsilon_p)]$</td>
</tr>
</tbody>
</table>

Figure 3.3: The analytical and fitted stress-strain curves of DP steel constituents using OriginLab software for DP#2 (a) ferrite phase and (b) martensite phase

A standard ASTM E8 specimen geometry was utilized in the quasi-static tension tests for design points under a strain rate of 0.005 sec$^{-1}$ with a uniform gauge length of 25 mm and thickness of 3 mm. On the other hand, at a high strain rate, a specimen of the Split-Hopkinson Tension Bar test was used with a normal gauge length of 5 mm and width of 3 mm as represented. A velocity boundary condition (nodal velocity $V$) was defined to one side of the tension specimen while the
opposite side was fixed. For a specified macroscopic strain rate, V is given by following equation [105]:

\[ V = \dot{\varepsilon} L_0 \]  \hspace{1cm} (3.29)

where \( \dot{\varepsilon} \) is the engineering strain rate and \( L_0 \) is the gauge length.

### 3.5 Results and Discussions

Each simulation point (design point) was performed according to conditions in the design matrix (see Table 3.3 below). The results of the micro-macro multiscale material modeling of DP steels and the RSM model are discussed in this section. The effects and interactions of microstructure parameters with the toughness, ultimate strength, and ductility of DP steels were investigated under different strain rates to optimize microscopic parameters at a specific strain rate.

#### 3.5.1 Model validation and mesh sensitivity

In finite element analysis, strain softening and localization is mesh sensitive. This is because the classical plasticity model does not have length scale and can only describe the mechanical behavior up to the onset of necking [82,109]. In this study, mesh size dependency analysis was conducted and compared with experimental results to estimate the accuracy of the simulation results. The experimental data that contained statistical quantitative metallography and the stress-strain curve of DP500 at a strain rate of 1110 and 0.001 sec\(^{-1}\) [1] were compared to the predicted numerical stress-strain curves at different mesh size as shown in Figure 3.4.

As can be seen in Figure 3.4, the simulation results are mesh independent and in good agreement with experimental results up to the onset of necking. This mesh size dependency was reduced by
using the elasto-viscoplastic framework presented in section 3.2.1 where viscosity was added to both the martensite and ferrite flow stress. This, however, does not significantly change the mechanical behavior (e.g. [82]).

**Figure 3.4:** Comparison between the experimental and numerical results at specific microstructure parameters ($d_f = 17.1 \, \mu m$, $d_m = 12.6 \, \mu m$, $V_m = 11.9\%$, and $C \, wt\% = 0.12$) [1], different mesh size, and strain rate.

### 3.5.2 Numerical flow curves of DP steels

The stress-strain curves for all the 30 design points in the design matrix (Table 3.3) are presented in Figure 3.5. It is obvious that the stress-strain curves are different due to changing microstructure parameters and strain rate.
Figure 3.5: Numerical stress-strain curves for all design points in the analysis matrix

Figure 3.6 presents representative samples of numerical true stress-strain curves of DP steels and their constituents for some design points (PD#1 and PD#9) in the design matrix. Also, the strain rate history that is applied is shown in Figure 3.6. It can be seen in Figure 3.6 that plastic deformation was controlled by ferrite phase and strengthening the steel was controlled by martensite phase. In both steels, martensite phase generally exhibited elastic behavior, which is in good agreement with the previous experimental results reported by Sun et al. [109].

In general, the precipitation hardening based on carbon content in the martensite phase is a significant strengthening mechanism that reinforces the DP steels; however, the strength of the ferrite phase depends on the ferrite grain size and the martensite volume fraction [2]. In order to compare the accuracy of the RSM modeling results with the traditional method, a sensitivity
analysis was carried out to investigate the effect of changing microstructure parameters on the flow stress of DP steels.

**Figure 3.6:** Flow curves of DP steels and their constituents predicted from the multiscale material model for (a) DP#1 and (b) DP#9
Consequently, the effect of each factor (microstructure parameter and strain rate) on the mechanical behavior of DP steels is conducted by changing the values of this individual factor while keeping the values of all other factors constant as shown in Figure 3.7.

**Figure 3.7**: The effect of each microstructure parameter on the flow stress (a) ferrite grain size, (b) martensite volume fraction, (c) carbon content, and (d) strain rate

Figure 3.7 reveals that the factors have various influences on the mechanical behavior of DP steels. The factors that have significant effects on the stress-strain curve of DP steels are the ferrite grain size ($d_f$), the martensite volume fraction ($V_m$) and the strain rate ($\dot{\varepsilon}$). However, a minor
effect on the mechanical behavior is found in the carbon content in DP steels (C wt%). Generally, increasing each factor separately while keeping the rest of the factors fixed increases the work hardening of DP steel as shown in Figure 3.8. Thus, the multiscale material model can predict any variation in the considered factors. Another key point to emphasize is that Figure 3.7 demonstrates the simple traditional methodology of the parametric study when changing one factor at a time while maintaining the other factors constantly. This traditional methodology is not capable of investigating the effects of interaction between factors on the performance of DP steels and achieving optimum factors setting. More interestingly, Figure 3.7 (a) clearly shows the influence of ferrite grain size on the mechanical behavior of DP steels as commonly observed (e.g., [89,110–112]), which reveals that when the ferrite grain size decreases, the strength of DP steels increases with slightly sacrificing the ductility. As follows from Figure 3.7 (b), the overall strength of DP steels and ductility increase with rising $V_m$, which is in agreement with that reported by Movahed et al. [101] and Abid et al. [22]. From the simulation results shown in Figure 3.7 (c), the carbon content in DP steels has slight significance on the mechanical behavior of DP steels. This effect can be attributed to the so-called geometrically necessary dislocations (GNDs) that form at the ferrite–martensite interfaces [104]. In addition, Figure 3.7 (d) illustrates how strain rate influences the overall strength of DP steels and demonstrates the obvious change in the stress–strain curves between low and high strain rates, which is in good agreement with the experimental results conducted by Wang et al. [81] and Alturk et al. [80]. Furthermore, Figure 3.8 demonstrates the effect of ferrite grain size on the ultimate strength, and ductility while maintaining other factors at constant values based on the simple traditional sensitivity analysis. Expected responses were found in Figure 3.8 where the ultimate strength obeyed the Hall-Petch effect, and ductility rises with increasing ferrite grain size.
Figure 3.8: The effect of ferrite grain size on ultimate strength and ductility for DP#8, DP#5, and DP#10 at constant other microstructure parameters ($V_m=25.15\%$, $C\text{ wt}\%=0.105\%$, and $\dot{\varepsilon}=250\text{ sec}^{-1}$)

3.5.3 Analysis of RSM model

The RSM consists of the design of experiments to achieve minimum variances of the responses, a regression surface fitting to find the approximate responses, and optimizations using the approximated responses. The complete quadratic model was chosen to analyze RSM using MINITAB software after adding tensile strength, and ductility as the responses in the designed analysis matrix as shown in Table 3.3. The RSM results were generated in the form of 2D and 3D surface charts of responses. Statistical assessments for RSM model were also presented as detailed in Table 3.4 and Table 3.5.

Table 3.4 illustrates the analysis of variance that summarizes the statistical significance of each factor on ultimate strength and ductility. Also, the coefficient column gives the coefficients for all the terms in the full regression equation in the RSM.
Table 3.3: Design of analysis matrix using MINITAB software with results of ultimate strength and ductility

<table>
<thead>
<tr>
<th>Design Points</th>
<th>Factors</th>
<th>Responses</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$d_f$ (µm)</td>
<td>$V_m$ (%)</td>
</tr>
<tr>
<td>DP#1</td>
<td>6.85</td>
<td>3.30</td>
</tr>
<tr>
<td>DP#2</td>
<td>6.85</td>
<td>47.00</td>
</tr>
<tr>
<td>DP#3</td>
<td>6.85</td>
<td>25.15</td>
</tr>
<tr>
<td>DP#4</td>
<td>6.85</td>
<td>25.15</td>
</tr>
<tr>
<td>DP#5</td>
<td>6.85</td>
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</tr>
<tr>
<td>DP#6</td>
<td>6.85</td>
<td>25.15</td>
</tr>
<tr>
<td>DP#7</td>
<td>6.85</td>
<td>25.15</td>
</tr>
<tr>
<td>DP#8</td>
<td>0.70</td>
<td>25.15</td>
</tr>
<tr>
<td>DP#9</td>
<td>6.85</td>
<td>25.15</td>
</tr>
<tr>
<td>DP#10</td>
<td>13.00</td>
<td>25.15</td>
</tr>
<tr>
<td>DP#11</td>
<td>0.70</td>
<td>3.30</td>
</tr>
<tr>
<td>DP#12</td>
<td>0.70</td>
<td>3.30</td>
</tr>
<tr>
<td>DP#13</td>
<td>0.70</td>
<td>47.00</td>
</tr>
<tr>
<td>DP#14</td>
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<td>25.15</td>
</tr>
<tr>
<td>DP#15</td>
<td>13.00</td>
<td>47.00</td>
</tr>
<tr>
<td>DP#16</td>
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<tr>
<td>DP#17</td>
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<td>47.00</td>
</tr>
<tr>
<td>DP#18</td>
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</tr>
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<tr>
<td>DP#20</td>
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</tr>
<tr>
<td>DP#21</td>
<td>0.70</td>
<td>47.00</td>
</tr>
<tr>
<td>DP#22</td>
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<td>3.30</td>
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<tr>
<td>DP#23</td>
<td>0.70</td>
<td>3.30</td>
</tr>
<tr>
<td>DP#24</td>
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<td>DP#28</td>
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</tr>
<tr>
<td>DP#29</td>
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</tr>
<tr>
<td>DP#30</td>
<td>13.00</td>
<td>3.30</td>
</tr>
</tbody>
</table>
Table 3.4 illustrates the analysis of variance that summarizes the statistical significance of each factor on ultimate strength and ductility. Also, the coefficient column gives the coefficients for all the terms in the full regression equation in the RSM. As can be seen in Table 3.4, the small p-values for ferrite grain size ($d_f$), martensite volume fraction ($V_m$), and strain rate ($\dot{\varepsilon}$) indicate that these effects are statistically significant on all responses. On the other hand, the carbon content in DP steels (C wt%) has slightly large p-values, which indicates that these effects are a certain trend toward quasi-significant. Moreover, the small p-values for the square term of ($d_f^2$), the interaction
term of \((d_f \times V_m)\), and the interaction term of \((d_f \times \dot{\varepsilon})\) indicate that these effects are statistically significant. In addition, Variance inflation factors (VIF’s) in Table 3.4 evaluate how much the variance of the predictable regression coefficients is inflated as compared to when the predictor variables are not linearly related. Thus, VIF values greater than 5-10 indicate that the regression coefficients are inadequately predictable due to severe multicollinearity.

Table 3.5: RSM model regression evaluation (Analysis of Variance (ANOVA) for ultimate strength and ductility)

<table>
<thead>
<tr>
<th>Term</th>
<th>(\sigma_u)</th>
<th>(\varepsilon_u)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-sq</td>
<td>97.21%</td>
<td>93.37%</td>
</tr>
<tr>
<td>R-sq (adj)</td>
<td>94.23%</td>
<td>86.26%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Source</th>
<th>DF</th>
<th>P-Value</th>
<th>DF</th>
<th>P-Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blocks</td>
<td>1</td>
<td>0.793</td>
<td>1</td>
<td>0.421</td>
</tr>
<tr>
<td>Linear</td>
<td>4</td>
<td>0.000</td>
<td>4</td>
<td>0.000</td>
</tr>
<tr>
<td>Square</td>
<td>4</td>
<td>0.003</td>
<td>4</td>
<td>0.001</td>
</tr>
<tr>
<td>2-Way Interaction</td>
<td>6</td>
<td>0.118</td>
<td>6</td>
<td>0.003</td>
</tr>
<tr>
<td>Lack-of-Fit</td>
<td>10</td>
<td>0.133</td>
<td>10</td>
<td>0.131</td>
</tr>
<tr>
<td>Pure Error</td>
<td>4</td>
<td>----</td>
<td>4</td>
<td>----</td>
</tr>
<tr>
<td>Total</td>
<td>29</td>
<td>----</td>
<td>29</td>
<td>----</td>
</tr>
</tbody>
</table>

Table 3.5 summarizes the linear terms, the squared terms, and the two way-interactions.

The small p-values for the two way-interactions, the linear terms, and the squared terms suggest that there is curvature in the response surface. For the full quadratic equation in the RSM model, the p-value for lack of fit is about 0.131 for three responses signifying that this model adequately
fits the simulations data of DP steels. The $R^2$ values signify that the predictors explain 97.21% of the variance in ultimate strength and 93.37% of the variance in ductility. In other words, the adjusted $R^2$ values indicate that the RSM model explains all the variability of the responses data around their mean. All these values suggest that the full quadratic equation in the RSM model fits the simulations data of DP steels well. Therefore, the verified regression equation of each response based on the most significant factors is as follows:

$$
\sigma_u = +780 - 59.6 (d_f) + 7.31(V_m) + 0.301 (\dot{\varepsilon}) + 3.026(d_f)^2 - 0.273 (d_f \times V_m) - 89.6 (d_f \times C \text{ wt%})
$$

(3.30)

$$
\varepsilon_u = -0.2327 + 1.24 \times 10^{-2} (d_f) + 2.74 \times 10^{-4}(V_m) - 3 \times 10^{-5} (\dot{\varepsilon}) - 6.67 \times 10^{-4}(d_f)^2 - 5.9 \times 10^{-5} (d_f \times V_m) + 4 \times 10^{-6}(d_f \times \dot{\varepsilon}) + 1 \times 10^{-6}(V_m \times \dot{\varepsilon})
$$

(3.31)

Since there are significant interaction terms, an interaction graph was used to take a closer look and estimate the presence of interaction among the considered factors. The Interaction graph that generates a matrix of interaction graphs for the considered factors for each response is shown in Figure 3.9.

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 Figure 3.9, the parallel lines in an interaction graph signify no interaction; however, the interaction exists in case the lines are not parallel status. The greater the difference in slope between the lines,
the higher the level of interaction. In the same figure, it can also be clearly seen that the interactions plots of carbon content (C wt%) with other factors do not have statistical significance.

**Figure 3.9**: Interaction Plots for (a) ultimate strength and (b) ductility (fitted means)

It is also obvious that the interaction graphs of the ductility mean show sufficient interaction between ferrite grain size ($d_r$) and other factors because the lines are not parallel as well as
martensite volume fraction ($V_m$) and other factors. The change in ultimate strength and ductility when it moves from the low level to the high level of $d_r$, $V_m$, and $\dot{\varepsilon}$ are about the same at levels of C wt%. Moreover, the change in ductility when it moves from the low level to the high level of $d_r$ is different depending on the level of other factors. Another key thing to remember is that these interaction graphs can be used to assess the main effects and interaction influences, provided that evaluating significance is determined by looking at the p-values for all interaction effects in the Analysis of Variance and the RSM model regression evaluation as shown in Table 3.4 and Table 3.5.

3.5.3.1 Parametric investigation

The parametric study was conducted by the RSM model, and the effects of the considered factors on each response as 6 plots of contours and 6 plots of three-dimensional plots were generated by MINITAB software. To give an illustration, Figures 3.10 and 3.11 show the 3D surface graphs of the factors effects on the ultimate strength and the ductility as responses. The provided plots in Figure 3.10 (a) shows clearly that the ultimate strength follows the Hall-Petch relationship; at the same time as, it has a slight variation with changing $V_m$. A glance at the ductility graph, Figure 3.11 (a), reveals that there is a peak (a clear optimum status) at the given level of $d_r$; on the other hand, the ductility approximately remains constant when $V_m$ changes at the high level of $d_r$ while it slightly increases at the low level of $d_r$. As is presented in Figure 3.10 (b), the ultimate strength remains constant with rising C wt% whereas it rises dramatically with increasing $\dot{\varepsilon}$. According to the ductility (Figure 3.11 (b)), at low level of $\dot{\varepsilon}$ the ductility increases rapidly with rising C wt%; while, at a high level of $\dot{\varepsilon}$ the ductility decreases with increasing $\dot{\varepsilon}$ until C wt% equals 0.12% and then it increases again. As shown in Figure 3.10 (c) and Figure 3.11 (c), the ultimate strength increase with going up both $V_m$ and $\dot{\varepsilon}$ and the higher strength value that is greater
than 1050 MPa is at a high level of \( V_m \) and \( \dot{\varepsilon} \). In addition, the ductility plot shows that the increase in the ductility from the low to the high level of \( V_m \) is greater at the high level of \( \dot{\varepsilon} \). By contrast, a change of ductility at low level of \( \dot{\varepsilon} \) is almost constant on changing \( V_m \).

The 3D surface plots in Figure 3.10 (d) and Figure 3.11 (d) illustrate that the carbon content in DP steels does not have any statistical significance on strength. However, the change in ductility from the low to the high level of C wt\% is greater at the high level of \( V_m \). Another key observation from Figure 3.11 (d) is that there is a minimum of ductility at mid-range of C wt\% (0.075 to 0.11 \%). The trend of the ultimate strength, Figure 3.10 (e), increases with rising \( \dot{\varepsilon} \) while the relationship of ultimate strength with ferrite grain size obviously obeys the Hall-Petch model. Not to mention, the given Figure 3.11 (e) shows a slight steadiness in the ductility with increasing \( \dot{\varepsilon} \). In Figure 3.10 (f) and Figure 3.11 (f), the relation of ultimate strength and ductility with ferrite grain size is similar to the trends in Figure 3.10 (a) and Figure 3.11 (a). Besides that, the change in the responses on carbon content shows a slight steadiness, which indicates that there is no statistical significance.

In order to sum up the results in Figures 3.10 and 3.11, Figure 3.12 shows the relationships between the responses and the considered factors, which represents each response means for each level of factors. The mean effect plot for the ultimate strength and ductility show that the strength increases gradually and the ductility increases slowly with rising \( V_m \) and \( \dot{\varepsilon} \) while they remain slightly constant with changing C wt\%. It may be seen clearly that the ductility rises significantly with increasing \( d_f \) and they reach their peak at \( d_f \) value equals 5 \( \mu \)m and 8 \( \mu \)m then they drop off. On the other hand, the ultimate strength decreases dramatically with increasing \( d_f \), which agrees with the literature and follows Hall-Petch role.
Figure 3.10: 3D surface plots for the ultimate strength with each two factors (a) C wt% = 0.105 and $\dot{\varepsilon} = 250 \text{ sec}^{-1}$, (b) $d_f = 6.85 \times 10^{-3} \text{ m}$ and $V_m = 25.15\%$, (c) C wt% = 0.105 and $d_f = 6.85 \times 10^{-3} \text{ m}$, (d) $d_f = 6.85 \times 10^{-3} \text{ m}$ and $\dot{\varepsilon} = 250 \text{ sec}^{-1}$, (e) C wt% = 0.105 and $V_m = 25.15\%$, and (f) $V_m = 25.15\%$ and $\dot{\varepsilon} = 250 \text{ sec}^{-1}$.
Figure 3.11: 3D surface plots for the ductility with each two factors (a) C wt% = 0.105 and $\dot{\varepsilon} = 250$ sec$^{-1}$, (b) $d_t = 6.85$ µm and $V_m = 25.15\%$, (c) C wt% = 0.105 and $d_t = 6.85$ µm, (d) $d_t = 6.85$ µm and $\dot{\varepsilon} = 250$ sec$^{-1}$, (e) C wt% = 0.105 and $V_m = 25.15\%$, and (f) $V_m = 25.15\%$ and $\dot{\varepsilon} = 250$ sec$^{-1}$
These results describe, for the first time, the complete statistical investigation of microstructure parameters effects and their roles in influencing the strain rate sensitivity of DP steels. As $V_m$ increases, the ultimate strength rises concurrently at the slight expense of ductility. However, this is expected and is commonly reported in the literature (e.g.,[22,113]).

Moreover, it can be seen from the results that $V_m$ has significant effect than the carbon content (C wt%) due to the direct connection between $V_m$ and C wt% in Eq’s (3.5) and (3.6). Thus, an increase in $V_m$ can implicitly influence the responses (the ultimate strength, and ductility) in two ways. Firstly, increasing $V_m$ increases the density of GNDs, which is mainly located at the ferrite-martensite interface and strengthens the ferrite phase. Secondly, as $V_m$ goes up in the number and

**Figure 3.12:** Mean effects plot for tensile toughness ultimate strength, and ductility (fitted means)
the size of the martensite particles and induces a decrease in the ferrite grain size (d_f). By growing the hardening of the ferrite phase, these two factors, in turn, improve the strength of DP steel [112] [114]. The results also show that due to the GND’s effect, the higher V_m and smaller d_f have a considerable influence on the ultimate strength of DP steels. The finding is quite surprising that the ductility has a relative maximum with changing d_f, which is different than the expected result that was found in Figure 3.8. According to Figure 3.11 (d), it has been found that the ductility rises with V_m at constant carbon content in DP steels. On the other hand, it increases with the carbon content at a fixed V_m as shown in Figure 3.11 (b) and (d), which agrees with experimental study performed by Pierman et al. [104]. As is presented in Figure 3.12, an increase in V_m rises ductility due to decrease carbon content in martensite phase which in turn leads to increasing ductility of the martensite phase. Hence, the increase in ductility of the martensite phase increases the overall ductility of the DP steels [101]. The small ferrite grain size (d_f) strengthens the ferrite phase, as well as the overall DP steel behavior. Interestingly, the small amount of carbon content (C wt%) in DP steel with high martensite volume fraction (V_m) increases the ductility slightly due to reducing martensitic carbon content, which causes the martensite phase to deform plastically during the deformation of the overall DP steel.

3.5.3.2 Optimizing microstructural engineering for DP steels

As mentioned in Section 3, the RSM model was utilized as a model for optimizing the microscopic parameters in the direction of different design requirements, which is metal forming processes. Maximizing the ultimate strength while keeping an acceptable ductility is required for forming purposes. Under this condition, the aim is to achieve the optimum d_f, V_m, and C wt% which, maximizes the responses within the considered ranges and the boundaries imposed by the process and applications. The RSM model optimizer tool illustrates how various factors affect the
predicted responses for the RSM model and presents the influence of the considered microstructure parameters on the responses, the ultimate strength and ductility of DP steel at certain strain rates. The simulation setting (the considered microstructure parameters) in the optimizer tool can be modified interactively to find the predicted responses for a specific input factor (or factors) setting of interest. The optimization plots as shown in Figures 3.13 and 3.14 show the influence of each variable (factor) (columns) on responses (composite desirability (rows)) at each chosen strain rate. The perpendicular red lines on the plots illustrate the existing parameter arrangement and the values in red shown at the top of a column exhibit the existing parameter value settings.

Figure 3.13: Optimization chart of microstructure parameters for the maximum ultimate strength and ductility of DP steel at strain rate 1 sec$^{-1}$
As is presented in Figure 3.13, the RSM model predicts that the ultimate strength and ductility at strain rate 1 sec\(^{-1}\) are maximized when all microscopic parameters settings are at \(d_{fr}=3.14\ \mu m\), \(V_m=47\%\), \(C\text{ wt}\%=0.15\%\). As can be seen from Figure 3.14, the setting of microstructure parameters \((d_{fr}=2.65\ \mu m,\ V_m=47\%,\ C\text{ wt}\%=0.10\%)\) at a strain rate of 0.14 sec\(^{-1}\) satisfies the effective and maximizing responses.

![Figure 3.14: Optimization chart of microstructure parameters for the maximum ultimate strength, and ductility of DP steel at strain rate 0.14 sec\(^{-1}\)](image)

The composite desirability (D) evaluates how the settings optimize a set of overall responses, which has a range of zero to one. Thus, the optimization results show that the composite desirability (0.821 and 0.801 for Figure 3.13 and 3.14 respectively) is close to 1, which indicates that the settings of microstructure parameters achieve satisfactory results for all responses as a
whole. Not to mention, there is a good match between the optimum setting of the martensite volume fraction (47%) and the work of Movahed et al. [101], where they reported that dual phase steels comprising 47% martensite volume fraction exhibit the optimum mechanical behavior in respect of tensile toughness, ultimate strength, and ductility. It has been found that the combined influence of the martensite volume fraction and the carbon content in DP steels has considerable influence on the responses with changing strain rate where the model changes the carbon content till achieving an optimum in all responses at a fixed volume fraction (47%). Comparing optimum results at a strain rate of 1 sec\(^{-1}\) with literature finding, the 47% optimum \(V_m\) and 2.6 µm optimum \(d_f\) is in agreement with previous studies [101] and [66].

3.6 Conclusions

In this work, the full micro-macro multiscale material modeling based on mean-field homogenization incremental formulation was adopted to predict the mechanical behavior of DP steels and investigate the effects of microscopic parameters using an elasto-viscoplastic constitutive model for each phase in the DP steel. To the best of our knowledge, this is the first study to use the response surface methodology (RSM) as a comprehensive statistical tool to investigate independently the key factors of microstructure that affects the overall behavior of DP steels under low and high strain rates conditions, which proves to be a powerful tool for studying these parameter effects on mechanical behavior of DP steels, and also to find the optimum microstructure parameters. The following are the conclusions obtained from this study:

1) Not only the proposed full micro-macro multiscale model was validated successfully under quasi-static and dynamic strain rates conditions for DP steels, but also the model contributes further understanding into improving strength and ductility of DP steels. Furthermore, the experimental behavior was modeled using a multiscale material model
and an elasto-viscoplastic constitutive equation with isotropic yield criterion. The simulation results of the experiments utilizing estimated material parameters presented an excellent agreement with experimental data in terms of mechanical behavior and mesh sensitivity.

2) The comprehensive statistical parametric study was used to study the interactions and effects of variations of microscopic parameters, which reveals that the microscopic parameters and their two-way interactions play an important role in the mechanical behavior of DP steels. It was shown that for these microstructure parameters, the strength, and formability of DP steels would be optimized. In other words, the findings suggest that this study of the microstructure parameters effects at various strain rate conditions could provide a method of optimizing not only the microscopic parameters, but also possible forming operations and collision-related data.

3) It is concluded that as the martensite volume fraction \( V_m \) increases the strength rise while enhancing the ductility slightly based on martensitic carbon content that is a function in \( V_m \) and \( C \) wt\% in DP steel as shown in the proposed Eq. (3.5) and (3.6). It has been demonstrated that the malleability slightly increases with rising martensite volume fraction \( V_m \) at a constant carbon content in DP steel \( (C \) wt\%) due to decreasing martensitic carbon content. Provided that through the virtual tensile test, the multiscale model presents non-trivial optima in the mechanical properties, which is found at 47% of martensite volume fraction \( V_m \) with changing other factors based on the design requirements and strain rate conditions.

4) Based on the simulation results, it can be concluded that the ultimate strength of DP steel increases significantly when ferrite grain size \( (d_f) \) decreases. Conversely, the ductility
increases gradually when ferrite grain size \((d_f)\) rises, and they reach their peak at different values of \(d_f\) and then decline. To understand this phenomenon, a physically based model with higher-order gradient plasticity theory needs to be implemented to explain and study this behavior and further effectively capture the size effect.

5) The quasistatic and dynamic stress-strain curves for the simulation results exhibit significant differences. The strain rate showed a remarkable effect on the ultimate strength and in some cases, a slight influence on ductility can be found.

6) To achieve the needs of steel manufacturers and the automobile designers to match the components requirements of DP steels in the automobile industry, the methodology presented in this paper provides a pathway to modify and optimize the setting of microstructure parameters interactively, to produce desirable materials for the intended application as well as towards various design requirements. Therefore, the desirable microscopic parameters of DP steels can be controlled by varying intercritical heat treatment temperatures [23].

**Acknowledgments**

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CHAPTER FOUR: KEY FACTORS INFLUENCING THE ENERGY ABSORPTION OF DUAL PHASE STEELS: MULTISCALE MATERIAL MODEL APPROACH AND MICROSTRUCTURE OPTIMIZATION

The increase in use of dual phase (DP) steels grades in the vehicle manufacturers, to enhance the crashworthiness resistance and reduce body car weight, requires the development of a clear understanding of the effect of various microstructural parameters on the energy absorption in these materials. Accordingly, DP steelmakers are interested in predicting the effective microscopic factors as well as optimizing microstructure properties for application in crash-relevant components of vehicle bodies. This study presents 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. Microstructures with varied ferrite grain sizes, martensite volume fractions, and carbon content in DP steels were studied. The impact of these microstructure features at different strain rates on energy absorption characteristics of DP Steels is investigated numerically using an elasto-viscoplastic constitutive model in the frame of a full micro-macro multiscale finite element method. A comprehensive statistical parametric study using response surface methodology (RSM) is performed to determine the optimum microstructure features for a required tensile toughness at different strain rates. The simulation 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 energy absorption characteristics of DP Steels and thus can be used to identify optimum microstructural conditions at different strain rate conditions.
4.1 Introduction

Automobile materials that are used in crash-related components of car bodies should meet specific standards that are required to pass collision-related tests before forming them into different vehicle components. It is well known that DP steel has a good combination of strength and ductility, and thus are increasingly being used by the automobile manufacturers in body car [80]. Furthermore, DP steels have been successfully used in vehicle parts that need crashworthiness resistance due to its good advantage in reducing car weight with enhancing passenger safety along with their benefits of lower manufacturing cost, which is utilized primarily for external body sheets in (doors, hoods, and fenders). The microstructure of DP steels includes martensite phase particles dispersed in the soft ferritic matrix. Generally, DP steels contain a purely ferrite phase as a matrix with about a 3.3–47% fraction of martensite islands spread as a hard phase over a matrix [48]. The effect of strain rate on the plastic behavior of DP steels under both quasi-static and dynamic loading conditions were investigated by several studies [1,2,24,32,50,66,80–95]. Conversely, the effect of the microstructure parameters and the role they play in influencing the plastic behavior of DP steels under low and high strain rates were examined by only a limited number of studies [1,2,24,32,50,76,80,81,84,85,87–89,92–95]. For instance, Wang et al. [81] studied experimentally the influence of the morphology and volume fraction of martensite phase on the dynamic mechanical properties of DP600, DP800, and DP1000 under high strain rates from 700 to 1000 sec\(^{-1}\). They found that tensile toughness of the DP600 declined with the rise of the strain rate; on the other hand, the tensile toughness of the DP800, the DP1000, and the M1200 improved as the strain rate increases. Alturk et al. [80] examined the impact of martensite phase content in DP980 and QP980 on the strain rate sensitivity at different strain rates 0.005 and 500 sec\(^{-1}\) that usually happens during a crash event. They reported that the energy absorption of DP980 improved
significantly with the increase in strain rates at values that are close to collision condition. Kim and Lee [87] investigated the effect of the morphology of martensite phase and martensite volume fraction on mechanical properties of DP steels under quasi-static and dynamic loading. Hwang et al. [89] studied the impact of microscopic parameters such as martensite volume fraction and ferrite grain size on dynamic torsional behavior and quasi-static tensile in DP steels. Other several researchers attempted to improve the mechanical properties of DP steels under different strain rate conditions by developing methods to obtain the optimum microstructure features and find a maximum tensile toughness and identification of the effective microstructure parameters [2,32,66,94,95].

In the last few years there has been a growing interest in finding guidelines for optimizing the microstructural features of DP steels in the direction of several purposes manufactured in terms of mechanical properties of specific final user, such as maximizing the tensile toughness characterizing the energy absorption for crashworthiness resistance or maximizing the strength with formability for metal forming process. However, very few publications can be found that address the issue of optimizing microscopic parameters of DP steels with different design requirements. For instance, Delincé et al. [19] provided, through a physically based model, parametric study on the effect of microstructure parameters on the flow stress of DP steels. The focus of this research was to provide guidelines for developing the microstructures based on ferrite grain size, martensite volume fraction, and carbon content toward differently formulated purposes regarding particular components mechanical properties, such as maximizing and characterizing the energy absorption or improving strength with flexibility. Nevertheless, a key limitation of these research is that it does not focus on a comprehensive statistical study of microstructural features effects and the roles they play in impacting the strain rate sensitivity of DP steels. Thus, increasing
attention has been received in recent years for developing an effective methodology for investigating the effects and interactions of microstructure properties of DP steels [115], and also various studies and processes have been attempted, but the multiscale modeling of multiphase material is still a nascent and an efficient endeavor. As a consequence, the authors have developed a new analytical methodology that can investigate the effect of microstructure properties, and can provide a comprehensive statistical parametric set of data which lead to an optimum microstructure characteristics [116]. In this study, the efficient analytical methodology that is presented in the authors’ pervious work [116] is used.

The methodology described in details in [115,116], utilizes micro-macro multiscale finite element modeling of DP steels along with a statistical and mathematical tool under low and high strain rates. A full micro-macro multiscale material modeling approach based on mean-field homogenization incremental formulation is developed to predict the flow stress of DP steels and examine the influences of the main microstructural features namely: ferrite grain size ($d_f$), martensite volume fraction ($V_m$), and Carbon content ($C_{wt\%}$) on the tensile toughness of DP steels under different strain rates ($\dot{\varepsilon}$). A dislocation density based nonlinear elastic-viscoplastic model that can predict the flow stress of DP steels under quasi-static and dynamic uniaxial loading conditions is developed, and the model is then used to generate a parametric study on the influence of microscopic parameters on the mechanical properties. This is followed by a systematic response surface methodology (RSM) investigation of the effect of microstructure factors on the energy absorption 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 tensile toughness at different strain rate conditions.
4.2 Methodology

4.2.1 Multiscale Material & Structure Modeling

Not only a multiscale material computational modeling is a necessity for studying the effect of microstructure parameters, but also it is essential for directing the material design of DP steels to enhance its tensile toughness for improving crash performance. For that reason, the mean-field homogenization (Digimat-MF) that is employed to predict the mechanical behavior of DP steels based on the constitutive equations of ferrite and martensite phase is used to link structural FEA software (LS-DYNA) through LS-DYNA user-defined material (UMAT) code. This model allows upstream and downstream two-scale material modeling where LS-DYNA is carried out at macro-scale, and for each time interval \((t_n, t_{n+1})\) at each integration point (IP) of the macro FE mesh, LS-DYNA/UMAT calls Digimat-MF through Digimat-CAE to perform the homogenization scheme of two phases (ferrite and martensite). The macro strain \((\bar{\varepsilon})\), materials constant, and history variables at \(t_n\) are passed by UMAT to Digimat-MF to compute the macro stress \((\bar{\sigma})\) and macro tangent moduli \((\bar{C})\) at \(t_{n+1}\). The micro-structure of two phases are not “seen” by LS-DYNA but only by Digimat-MF, which takes into account each integration point to be the center of a representative volume element (RVE) which contains the heterogeneous micro-structure of two phases as shown in Figure 4.1.
4.2.2 Constitutive equations description and parameter identification

Ferrite and martensite flow stress are described by using a dislocation density constitutive formulation where the typical relationship of the flow stress based on dislocation density can be written as \([2, 25, 26, 51, 64, 70, 73-75, 96]\):

\[
\sigma_{flow}^{f,m} = \sigma_{y0}^{f,m} + \alpha M \mu b \sqrt{\rho}^{f,m}, \text{ } f \text{ and } m \text{ refer to ferrite and martensite phase}
\]  

(4.1)
where $\alpha$ is a constant, $M$ is the Taylor factor, $\mu$ is the shear modulus, $b$ is the Burger’s vector, and $\rho$ is the dislocation density. The $\sigma_{y0}^{f,m}$ is initial yield and consists of the following hardening components:

$$\sigma_{y0}^{f,m} = \sigma_g^{f,m} + \Delta\sigma_c^{f,m} + \sigma_s$$  \hspace{1cm} (4.2)

where $\sigma_g$ is grain size effect that is expressed by the Hall-Petch model:

$$\sigma_g^{f,m} = \frac{K_{HP}}{\sqrt{d_{f,m}}}$$  \hspace{1cm} (4.3)

Here, $K_{HP}$ is the Hall-Petch constant and $d_{f\text{ or } m}$ is grain size of ferrite or martensite phase.

The $\Delta\sigma_c$ is precipitation hardening based on carbon content in solid solution. In the case of ferrite, it is $[2,51,70,97]$:

$$\Delta\sigma_c^f = 5000 \times \%C_{ss}^f$$  \hspace{1cm} (4.4)

In the case of martensite, the relationship between the martensite precipitation hardening and the carbon content in martensite phase is a linear relationship, which agrees with experimental results obtained on martensite $[66,98,99]$:

$$\Delta\sigma_c^m = \sigma_{y0}^m|_{\%C_{ss}=0} + \text{Cs} \times \%C_{ss}^m$$  \hspace{1cm} (4.5)

where $\sigma_{y0}^m|_{\%C_{ss}=0}$ is the initial yield stress of martensite at zero carbon content, which is the extrapolated from experimental results in Ref [98] at carbon-free. Cs is the carbon sensitivity and $\%C_{ss}^f$ and $\%C_{ss}^m$ is wt.% carbon content in solid solution in ferrite and martensite, respectively.
The carbon content in the ferrite phase is assumed to be 0.02%, which is the solubility limit for carbon in ferrite at room temperature. Even though the increase in the flow and tensile strengths with increasing martensite volume fraction at a defined carbon content in the martensite phase is noted and broadly reported (e.g. [100–102], to cite only a few), the law of mixture can be used to calculate the carbon content in the martensite phase based on the carbon content in DP steel [70]. It can be described as:

\[
\%C_{ss}^{DP} = \%C_{ss}^f \times V_f + \%C_{ss}^m \times V_m
\]  

(4.6)

where \(\%C_{ss}^{DP}\) is the nominal carbon composition of the DP steel, and \(V_f\) and \(V_m\) are the ferrite volume fraction and martensite volume fraction, respectively. This is a simplification, but it is considered as a reasonably suitable approximation.

The solid solution stress \(\sigma_s\) is the contribution of the solid solution hardening and effect of alloying elements in solid solution and it can be described as [2,51,64,70]:

\[
\sigma_0 \text{(in MPa)} = 77 + 80\%\text{Mn} + 750\%\text{P} + 60\%\text{Si} + 80\%\text{Cu} + 45\%\text{Ni} + 60\%\text{Cr} + 11\%\text{Mo} + 5000\%\text{N}
\]  

(4.7)

In this model, the solid solution stress is calculated at the middle of the alloying elements ranges in DP steels, which is approximately 274 MPa.

According to the Mecking-Kocks theory, the rate of dislocation density evolution to shear strain during the deformation is the result of the competition between the rate of production of dislocation and the annihilation rate of dislocation [2]. Rodriguez and Gutierrez [103] further developed this concept for the ferritic and martensitic phase; thus, the effective stress-strain relation is given by:
\[ \Delta \sigma = \alpha \mu \sqrt{b} \sqrt{\frac{1 - \exp(-Mk_r \varepsilon)}{k_r L}} \]  

(4.8)

where \( L \) is the dislocation mean free path and \( k_r \) is a constant. Once the description of the three terms in Eq (4.1) has been defined, the complete methodology for determining the flow stress of each phase in the DP steel is:

\[ \sigma_{f,\text{flow}} \equiv \sigma_{y0} + \alpha \mu \sqrt{b} \sqrt{\frac{1 - \exp(-Mk_r \varepsilon)}{k_r L}} \]  

(4.9)

where \( \sigma_{f,\text{flow}} \) and \( \varepsilon \) are responsible for the true flow stress (von Mises stress) and true strain, respectively.

In this study, an appropriate constitutive equation of each phase is used to conduct a finite element analysis of the quasi-static and dynamic tensile experiments on the DP steel in the Digimat-MF model. Through this equation, an elasto-viscoplastic (EVP) constitutive model is utilized to describe the flow stress of DP Steel at different strain rates [22]. In this model, von Mises plasticity model, assuming isothermal conditions and neglecting temperature increase due to plastic dissipation, associated flow rule, combined power law isotropic hardening, and strain-rate effects are included, and is given by the following equations:

\[ \sigma_{eq} = \sigma_{y0} + K^f \varepsilon_{p}^n \]  

(4.10)

with
\[
\sigma_{eq}^f = \sqrt{\frac{2}{3} (S^f : S^f)} , \quad S^f = \sigma^f - \frac{1}{3} \sigma_{kk}^f I 
\] (4.11)

\[
\sigma_{eq}^m = \sigma_{y0}^m + R \left[ 1 - \exp(m \varepsilon_p) \right] 
\] (4.12)

The evolution of the viscoplastic flow rule obeys the following flow rule:

\[
D_{vp}^f = \frac{3}{2} \frac{\dot{\varepsilon}_{vp}^f}{\sigma_{eq}^f} S^f 
\] (4.13)

\[
\dot{\varepsilon}_{vp}^f = \frac{\sigma_{y0}^f}{\dot{\varepsilon}_{vp}^f} \left[ \frac{\sigma_{eq}^f - \sigma_{y0}^f - K^f n^f \varepsilon_p^f}{\sigma_{eq}^f} \right]^{m^*} 
\] (4.14)

\( K^f, n^f, R \) and \( m \) are the ferrite hardening modulus, the ferrite strain hardening exponent, the martensite hardening modulus and the martensite strain hardening exponent respectively, which are obtained by curve fitting equation (4.10) and (4.12) to the data obtained from Eq (4.9). The other parameter values that are used for the ferrite and martensite phases in multiscale material model simulation are listed in Table 4.1. Another key feature is that the flow stress of martensite phase is described by using exponential law (Eq (4.12)), which is recommended by Digimat for material exhibits a horizontal plateau in the stress-strain curve, and was used successfully by Pierman et al. [76] to fit experimental data of bulk martensite samples. Additionally, in this study, an increase in temperature is assumed to be negligible, and the isothermal condition in this model is considered based on experimental work that was conducted by Tarigopula et al. [105]. They found that the temperature was gradually changed from the room temperature to approximately
60K in the region of large strain at a strain rate of 445 sec\(^{-1}\) for DP800, which is neglected and considered a moderate temperature rise.

**Table 4.1**: Description of the different materials parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Magnitude (Unite)</th>
<th>Used in Eq.</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic modulus</td>
<td>E</td>
<td>210 (GPa)</td>
<td>---</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Taylor constant</td>
<td>(\alpha)</td>
<td>0.33</td>
<td>(1), (9), (10)</td>
<td></td>
</tr>
<tr>
<td>Taylor factor</td>
<td>M</td>
<td>3</td>
<td>(1), (9), (10)</td>
<td></td>
</tr>
<tr>
<td>Shear modulus</td>
<td>(\mu)</td>
<td>80000 (MPa)</td>
<td>(1), (9), (10)</td>
<td></td>
</tr>
<tr>
<td>Magnitude of the Burgers vector</td>
<td>(b)</td>
<td>2.5x10(^{-10}) (m)</td>
<td>(1), (8), (9), (10)</td>
<td></td>
</tr>
<tr>
<td>Hall–Petch constant</td>
<td>(K_{HP})</td>
<td>150 (MPa(\sqrt{\text{mm}}))</td>
<td>(3)</td>
<td>[66]</td>
</tr>
<tr>
<td>Carbon content in ferrite</td>
<td>(%C_{ss})</td>
<td>0.02 (wt %)</td>
<td>(4)</td>
<td>[100,101]</td>
</tr>
<tr>
<td>Initial yield stress of martensite phase</td>
<td>(\sigma_{y0}^m)</td>
<td>1250 (MPa)</td>
<td>(5)</td>
<td>[66]</td>
</tr>
<tr>
<td>Carbon sensitivity constant</td>
<td>(C_s)</td>
<td>1600 (MPa/wt %)</td>
<td>(5)</td>
<td></td>
</tr>
<tr>
<td>Peierls stress</td>
<td>(\sigma_0)</td>
<td>274 (MPa)</td>
<td>(7)</td>
<td></td>
</tr>
<tr>
<td>Dislocation mean free path in ferrite</td>
<td>(L)</td>
<td>(d_r) ((\mu)m)</td>
<td>(8), (9), (10)</td>
<td></td>
</tr>
<tr>
<td>Dislocation mean free path in martensite</td>
<td></td>
<td>3.8x10(^{-8}) (m)</td>
<td>(8), (9), (10)</td>
<td>[2,51,70,77]</td>
</tr>
<tr>
<td>Recovery rate in ferrite</td>
<td>(k_r)</td>
<td>10(^{-5}/d_r)</td>
<td>(8), (9), (10)</td>
<td></td>
</tr>
<tr>
<td>Recovery rate in martensite</td>
<td></td>
<td>41</td>
<td>(8), (9), (10)</td>
<td></td>
</tr>
<tr>
<td>Viscoplastic coefficient</td>
<td>(\beta)</td>
<td>1000 (MPa.sec)</td>
<td>(14)</td>
<td>[22]</td>
</tr>
<tr>
<td>Strain rate</td>
<td>(m^*)</td>
<td>1</td>
<td>(14)</td>
<td>[22]</td>
</tr>
</tbody>
</table>

### 4.2.3 Homogenization technique

Homogenization schemes are commonly based on the hypothesis of a representative volume element (RVE), which represents a macroscopic point in the multiphase materials (i.e., an IP in a Finite Element simulation) as a finite inhomogeneous size that is representative of a microscopic point in the multiphase materials. Mean-field homogenization (MFH) model that aims to calculate the volume average of stress and strain states at the macro scale (RVE) and microscale.
(each phase) was utilized [106]. In a multiscale material model, the macro strain is known at each macroscopic point $\bar{x}$, which is the center of RVE of the multiphase material, DP steel.

Three general procedures that describe the homogenization scheme in the multiscale material model are shown in Figure 4.2. The allocation procedure is the first step, where the given strain is allocated for each phase (ferrite and martensite phase). The second procedure is microscopic stress computation for each phase based on the defined constitutive equations in the previous section. In the third procedure, a particular homogenization technique is applied to average the microscopic stress field and to obtain a macroscopic stress field. It can be seen that the multiscale model of multiphase materials relies explicitly on the behavior of the microstructure constituents, the current shape of inclusion and its orientation.

**Figure 4.2:** General homogenization scheme
For multiphase materials including only two phases such as DP steels, a Mori-Tanaka model has been proposed by Tanaka and Mori [71]. In this model, they supposed that the inclusions in the RVE undergo the matrix strain as the far-field strain in the Eshelby’s solution. This leads us to that the Mori-Tanaka model is attractive for multiphase materials like DP steels. In addition, it has a physical explanation, which makes each inclusion acts in the same way as an isolated inclusion in the matrix seeing as a far strain field [38,71,106,107].

4.2.4 Response Surface Methodology (RSM)

RSM is employed to examine the relationship between a response variable and a set of factors [78,108]. This RSM model initially allowed us to design the experiment effectively, and then provided data for a parametric study and optimization. In this study, RSM was used as a statistical design of simulation processes, which refers to the method of arranging the tests so that the appropriate data can be examined statistically. The required analysis points (the simulation settings) within specified ranges of microstructure parameters and strain rate were defined by using RSM. The ranges of microstructure parameters (d_r range of 0.7 – 13 µm, V_m range of 3.3 – 47%, and C wt% ranges 0.06 – 0.15 wt % in DP steels) were estimated based on the previous literature review and a few preliminary trials. In addition, strain rate range ( \dot{\varepsilon} range of 0.005-500 sec^{-1}) were chosen according to their lifetime of automotive materials particularly a collision events [80]. 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.

The complete quadratic polynomial regression model as shown in Eq (4.15) was determined for predicting the response variable (ℱ) regarding the independent variables (X_1, X_2, X_3, X_4), that are the microstructure parameters and strain rate.
To evaluate the crash resistance performance of DP steels, a tensile toughness (i.e., the energy absorbed by DP steels at certain points of deformation) provides valuable data, and that is a strong indication to determine a good strength/ductility combination. A good toughness means a high strength and a high ductility, and vice versa. Material toughness is measured by computing the area under the stress-strain curve for tensile test, and it is expressed in tensile toughness (energy units/volume) [79]. Consequently, the multi-scale material modeling was performed according to the analysis design matrix listed in Table 4.2 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. The RSM model results are presented in the form of 3D and 2D diagrams, which exhibit how the response variable is a function of four factors based on a model regression as shown in Eq (4.15).

\[
F = a_0 + a_1 X_1 + a_2 X_2 + a_3 X_3 + a_4 X_4 + a_{11} X_1^2 + a_{22} X_2^2 + a_{33} X_3^2 \\
+ a_{44} X_4^2 + a_{12} X_1 X_2 + a_{13} X_1 X_3 + a_{14} X_1 X_4 + a_{23} X_2 X_3 \\
+ a_{24} X_2 X_4 + a_{34} X_3 X_4 \quad (4.15)
\]

4.3 Results and discussion

Each simulation point (design point) was performed according to strain rate conditions in the design matrix. The results of the micro-macro multiscale material modeling of DP steels and the RSM model are discussed in this section. The effects and interactions of microstructure parameters with the toughness, ultimate strength, and ductility of DP steels were investigated under different strain rates to optimize microscopic parameters at a specific strain rate. The entire modeling procedure was accomplished using MINITAB (RSM), OriginLab (Data management tool), Digimat software (Mean field homogenization), and LS-DYNA (FE software). The micro-macro multi-scale material model of the mechanical behavior of DP steels was conducted in six procedures:
Table 4.2: Design of analysis matrix using MINITAB software

<table>
<thead>
<tr>
<th>Design Points (Run order)</th>
<th>Factors</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>d$_f$ (µm)</td>
</tr>
<tr>
<td>DP#1</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#2</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#3</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#4</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#5</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#6</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#7</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#8</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#9</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#10</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#11</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#12</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#13</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#14</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#15</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#16</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#17</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#18</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#19</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#20</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#21</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#22</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#23</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#24</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#25</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#26</td>
<td>13.00</td>
</tr>
<tr>
<td>DP#27</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#28</td>
<td>6.85</td>
</tr>
<tr>
<td>DP#29</td>
<td>0.70</td>
</tr>
<tr>
<td>DP#30</td>
<td>13.00</td>
</tr>
</tbody>
</table>

1) An analysis matrix that contains design points was designed and created using Minitab as mentioned in section 4.2.4.
2) An appropriate flow behavior of the ferrite and martensite phases were determined according to Eq (4.10) and the required parameters that are listed in Table 4.1.

3) The OriginLab software was conducted to fit equation (4.10) and (4.12) to the analytical flow stress of ferrite and martensite phase (Eq (4.9)) to define mechanical constants of constituents for all design points, for example, shown in Table 4.3 and Figure 4.3.

4) Flow curves of two phases for each design point were introduced to Digimat-MF, and coupling Digimat-MF to LS-DYNA via UMAT/Digimat-CAE was performed, and loading and boundary conditions were defined in LS-DYNA.

5) The flow curve of the micro-macro multi-scale material model for each design point in coupling Digimat-MF to LS-DYNA was obtained, and toughness was calculated for each flow curve using OriginLab.

6) An analysis of the RSM model by adding tensile toughness, ultimate strength and ductility for each design point to the design of the analysis matrix was carried out to obtain 2D contour plots, 3D surface plots, and the microstructure parameters optimization.

**Table 4.3**: The analytical and fitted flow stress of DP steel constituents for design points (2)

<table>
<thead>
<tr>
<th>DP#</th>
<th>Flow stress according to Eq. (4.9)</th>
<th>Flow stress according to fitted Eq. (4.10) and (4.12)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DP#2</td>
<td>( \sigma_{\text{flow}}^f = 332 + 1.25 \times \sqrt{(1 - \exp(-4.38\varepsilon_p))/(10^{-5})} )</td>
<td>( \sigma_{\text{flow}}^f = 332 + 659\varepsilon_p^{0.451} )</td>
</tr>
<tr>
<td></td>
<td>( \sigma_{\text{flow}}^m = 1978 + 1.25 \times \sqrt{(1 - \exp(-123\varepsilon_p))/(1.56 \times 10^{-6})} )</td>
<td>( \sigma_{\text{flow}}^m = 1978 + 975[1 - \exp(-309\varepsilon_p)] )</td>
</tr>
</tbody>
</table>
Figure 4.3: The analytical and fitted stress-strain curves of DP steel constituents using OriginLab software for DP#2 (a) ferrite phase and (b) martensite phase

Specimen dimensions of a standard ASTM E8 and a Split-Hopkinson tension bar [105] were used to simulate tension tests under quasi-static and dynamic strain rate to determine the flow stress for each design point. Specimen dimensions that were used in the simulation were identical to those that were used in the experimental tests as shown in Figure 4.4.

Figure 4.4: Dimension of the specimen (a) a standard ASTM E8 specimen and (b), a specimen of the Split-Hopkinson Tension Bar test
A velocity boundary condition (nodal velocity $V$) was defined to one side of the tension specimen while the opposite side was fixed. For a specified macroscopic strain rate, $V$ is given by following equation [105]:

$$\Delta V = \dot{\varepsilon} L_0$$

(4.16)

where $\dot{\varepsilon}$ is the engineering strain rate and $L_0$ is the gauge length.

Strain softening and localization is mesh sensitive in finite element analysis, which is caused by the classical plasticity model that does not have length scale and can only describe the mechanical behavior up to the onset of necking [82,109]. In order to verify the mesh sensitive, mesh size dependency analysis was conducted and compared with experimental results to estimate the accuracy of the numerical results. The experimental data that contained statistical quantitative metallography and the stress-strain curve of DP500 at a strain rate of 1110 and 0.001 sec$^{-1}$ [1] were compared to the predicted numerical stress-strain curves at different mesh size as shown in Figure 4.5.

The Figure 4.5 shows that the numerical results are mesh independent except at a high strain rate that slightly meshes dependent. Having said that, all numerical results are acceptable accuracy by comparing with experimental results up to the onset of necking. This mesh size dependency was reduced by using the elasto-viscoplastic framework presented in section 4.2.2 where viscosity was added to both the martensite and ferrite flow stress. This, however, does not significantly change the mechanical behavior (e.g. [82]). On the other hand, when the classical plasticity model was used as shown in Figure 4.6, the simulation results were affected significantly by mesh density, and the onset of necking was achieved with the increased refinement of finite element meshing, and the sharpest post-critical incline as well (e.g. [82,109]).
Figure 4.5: Comparison between the experimental and numerical results at specific microstructure parameters ($d_f = 17.1 \, \mu m$, $d_m = 12.6 \, \mu m$, $V_m = 11.9\%$, and $C \text{ wt}\% = 0.12$) [1], different mesh size, and strain rate

Figure 4.6: Comparison between the experimental and numerical results at different mesh size, microstructure parameters ($d_f = 5.45 \, \mu m$, $d_m = 0.9 \, \mu m$, $V_m = 9\%$, and $C \text{ wt}\% = 0.063$) and at $\dot{\varepsilon} = 0.14 \, \text{sec}^{-1}$ [2]
4.3.1 Numerical stress-strain relations and microstructural analysis

The Multiscale material modeling using coupled Digimat with LS-DYNA was conducted on all design points in the design matrix presented in Table 4.2 in order to simulate the flow stress of DP steels. The stress-strain curves for all 30 design points in the design matrix are presented in Figure 4.7. It is understandable that the stress-strain curves are different due to varying microscopic features and strain rate according to the considered design matrix in Table 4.2.

![Graph](image_url)

**Figure 4.7:** Numerical stress-strain curves for all design points in the analysis matrix presented in Table 2

Figure 4.8 gives an example of the numerical true stress-strain curves of DP steels and their constituents for two design points (PD#1 and PD#9) in the analysis design matrix, as well as strain rate that is applied to a specimen of DP#1 and DP#9. It can be seen in Figure 4.8 that strengthening
DP steel was controlled by martensite phase and plastic deformation was controlled by ferrite phase. In the simulation results, martensite phase generally showed elastic behavior, which is in good agreement with the previous experimental results reported by Sun et al. [109].

![Numerical flow stress curves of DP steels and their constituents for (a) DP#1 and (b) DP#9](image)

**Figure 4.8:** Numerical flow stress curves of DP steels and their constituents for (a) DP#1 and (b) DP#9

Generally, a significant strengthening mechanism that strengthens the DP steels comes first from precipitating carbon atoms in the martensite phase, and second from the strength of the ferrite phase that depends on the ferrite grain size and the martensite volume fraction [2].

In order to compare the accuracy of the RSM modeling results with a traditional parametric study, a simple traditional sensitivity analysis was conducted to examine the influence of microscopic features and strain rates on the tensile toughness of DP steels. Thus, the influence of each factor (microstructure parameter and strain rate) on the energy absorption of DP steels is carried out by changing the values of this individual factor while keeping the values of all other factors constant as shown in Figure 4.9.
Figure 4.9: The effect of each microstructure parameter on the tensile toughness of DP steel (a) ferrite grain size, (b) martensite volume fraction, (c) strain rate, and (d) carbon content

Figure 4.9 reveals that the factors have various influences on the energy absorption of DP steels. Furthermore, the factors that have significant effects on the tensile toughness of DP steels are the martensite volume fraction ($V_m$), the ferrite grain size ($d_f$), and the strain rate ($\dot{\varepsilon}$). However, the minor impact on the toughness is found in the carbon content in DP steels ($C$ wt%).

In general, increasing each factor separately while maintaining the rest of the factors fixed increases the energy absorption capacity of DP steels as shown in Figure 4.9, which indicates that the multiscale material model can predict any variation in the tensile toughness due to change in considered factors. More interestingly, Figure 4.9 (a) clearly presents the influence of ferrite grain size on the energy absorption capacity of DP steels as commonly observed (e.g., [79,117]), which
reveals that reducing ferrite grain size resulted in the upsurge of tensile strength, yield stress, and the work hardening of DP steels; on the other hand, it decreases the yield stress to tensile strength ratio. As follows from Figure 4.9 (b), the tensile toughness increases with rising $V_m$, which is in agreement with that reported by Movahed et al. [101] and Bag et al. [118]. Figure 4.9 (c) illustrates how strain rate influences the tensile toughness of DP steels and demonstrates the obvious change in the energy absorption capacity between quasi-static and dynamic loading condition, which is in good agreement with the experimental results conducted by Wang et al. [81] and Alturk et al. [80]. In addition, Figure 4.9 (d) shows that the carbon content in DP steels has slight significance on the energy absorption capacity of DP steels. As mentioned previously, the results in Figure 4.9 demonstrates the simple traditional methodology of the parametric study when changing one factor at a time while maintaining the other factors constantly, which is not capable of investigating the effects of interaction between factors on the energy absorption of DP steels and achieving optimum factors setting.

To give another illustration of the simple traditional sensitivity analysis, Figure 4.10 shows the influence of ferrite grain size on the tensile toughness, ultimate strength, and ductility while maintaining other factors at constant values. Expected results were found in Figure 4.10 where the energy absorption capacity and ductility increase with rising the ferrite grain size and the ultimate strength obviously obeyed Hall-Petch relation. Not only did Figure 4.10 reveals the expected results, but it also gives us an indication that the tensile toughness is a good measurement for a good combination of strength and ductility, which agrees with the preexisting studies (e.g., [1,80,81]).
Figure 4.10: The effect of ferrite grain size on tensile toughness, ultimate strength, and ductility for DP#8, DP#5, and DP#10 at constant other microstructure parameters (V_m = 25.15%, C wt% = 0.105%, and \( \dot{\varepsilon} = 250 \text{ sec}^{-1} \))

4.3.2 Analysis of RSM model

Tensile toughness for each design point was computed using the OriginLab software in order to determine responses in the RSM model, which is measured by calculating the area under stress-strain curves from strain range from 0 to strain at ultimate strength (\( \varepsilon_u \)). Coupled with Figure 4.10, tensile toughness relies on both ultimate strength and ductility, which is problematical to predict its discrepancy by straightforwardly observing at the variations in tensile strength and ductility in the stress-strain curves; their combined influence is to be of importance. After adding tensile toughness as the response in the designed analysis matrix as shown in Table 4.4 and
choosing the full quadratic equation to express the response, the RSM model was conducted using MINITAB software.

The RSM results were generated in the form of 2D and 3D surface charts of responses. Important statistical assessments for RSM model were also presented as detailed in Table 4.5.

Table 4.4: Design of analysis matrix using MINITAB software with results of tensile toughness
Table 4.5: Analysis of Variance (ANOVA) results of the statistical significance of each factor for response (Estimated Regression Coefficients)

<table>
<thead>
<tr>
<th>Term</th>
<th>P-Value</th>
<th>Coeff.</th>
<th>VIF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Constant</td>
<td>0.000</td>
<td>+ 133.7</td>
<td>-----</td>
</tr>
<tr>
<td>$d_r$</td>
<td>0.015</td>
<td>+ 7.64</td>
<td>1.00</td>
</tr>
<tr>
<td>$V_m$</td>
<td>0.000</td>
<td>+ 1.40</td>
<td>1.00</td>
</tr>
<tr>
<td>C wt%</td>
<td>0.580</td>
<td>+ 59</td>
<td>1.00</td>
</tr>
<tr>
<td>$\dot{\varepsilon}$</td>
<td>0.000</td>
<td>- 0.014</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_r * d_r$</td>
<td>0.087</td>
<td>- 0.605</td>
<td>2.84</td>
</tr>
<tr>
<td>$V_m * V_m$</td>
<td>0.496</td>
<td>+ 0.0182</td>
<td>2.84</td>
</tr>
<tr>
<td>C wt%*C wt%</td>
<td>0.938</td>
<td>+ 488</td>
<td>2.84</td>
</tr>
<tr>
<td>$\dot{\varepsilon} * \dot{\varepsilon}$</td>
<td>0.557</td>
<td>+ 0.000120</td>
<td>2.84</td>
</tr>
<tr>
<td>$d_r * V_m$</td>
<td>0.006</td>
<td>- 0.1185</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_r * C wt%$</td>
<td>0.631</td>
<td>- 8.8</td>
<td>1.00</td>
</tr>
<tr>
<td>$d_r * \dot{\varepsilon}$</td>
<td>0.009</td>
<td>+ 0.00980</td>
<td>1.00</td>
</tr>
<tr>
<td>$V_m * C wt%$</td>
<td>0.487</td>
<td>- 3.60</td>
<td>1.00</td>
</tr>
<tr>
<td>$V_m * \dot{\varepsilon}$</td>
<td>0.076</td>
<td>+ 0.001739</td>
<td>1.00</td>
</tr>
<tr>
<td>C wt% * $\dot{\varepsilon}$</td>
<td>0.539</td>
<td>- 0.277</td>
<td>1.00</td>
</tr>
<tr>
<td>Blocks</td>
<td>0.355</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Linear</td>
<td>0.000</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Square</td>
<td>0.493</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>2-Way Interaction</td>
<td>0.014</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Lack-of-Fit</td>
<td>0.130</td>
<td>--</td>
<td>--</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>R-sq</th>
<th>R-sq (adj)</th>
</tr>
</thead>
<tbody>
<tr>
<td>90.83%</td>
<td>81.01%</td>
</tr>
</tbody>
</table>
Table 4.5 illustrates the analysis of variance that summarizes the statistical significance of each factor and the linear terms, the squared terms, and the two way-interactions on the energy absorption capacity of DP steels. As well, the coefficient column gives the coefficients for all the terms in the full regression equation in the RSM. As can be seen in Table 4.5, the small p-values for ferrite grain size (dF), martensite volume fraction (Vm), and strain rate (ε̇) indicate that these effects are statistically significant on tensile toughness; as well as, the two way-interactions and the linear terms suggest that there is curvature in the response surface. On the other hand, the carbon content in DP steels (C wt%) has slightly large p-values, which indicates that these effects are a certain trend toward quasi-significant. Moreover, the small p-values for the interaction term of (dF * Vm), and the interaction term of (dF * ε̇) indicate that these interaction influences are statistically significant. In addition, Variance inflation factors (VIF’s) in Table 4.5 evaluate how much the variance of the predictable regression coefficients is inflated as compared to when the predictor variables are not linearly related. Thus, VIF values greater than 5-10 indicate that the regression coefficients are inadequately predictable due to severe multicollinearity. According to the p-value for lack of fit, the RSM model adequately fits the simulations data of DP steels. The R^2 values signify that the predictors explain 90.83% of the variance in tensile toughness. In other words, the adjusted R^2 values indicate that the RSM model explains all the variability of the response data around their mean.

Likewise, the residual charts, Figure 4.11, that describe how well they fit the simulations data of DP steels do not signify any problems with the RSM model. The normal probability graph proves an approximately linear pattern consistent with a normal distribution. Similarly, the residual - fitted values graph presents a random pattern, which proposes that the residuals have constant variance even though this graph shows one potential outlier. Also, the histogram presents one potential
outlier in the data; however, the normal probability graph assesses linear pattern consistent with a normal distribution. All these important statistical assessments suggest that the full quadratic equation in the RSM model fits the simulations data of DP steels well. Therefore, the verified regression equation of response based on the most significant factors is as follows:

\[
\text{Toughness } \left( \frac{\text{MJ}}{\text{m}^3} \right) = + 133.7 + 7.64(d_f) + 1.40(V_m) - 0.014(\varepsilon') - 0.605(d_f)^2 \\
- 0.1185(d_f \times V_m) + 0.00980(d_f \times \varepsilon') + 0.001739(V_m \times \varepsilon')
\]  

(4.17)

**Figure 4.11:** The residual plots for response, tensile toughness

Since the interaction term for response is significant, an interaction graph was used to take a closer look and estimate the presence of interaction among the considered factors. The Interaction graph that generates a matrix of interaction graphs for the considered factors is shown in Figure 4.12. 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 Figure 4.12, the parallel lines in an interaction graph signify no interaction; however, the interaction exists in case the lines are not parallel status. The greater the difference in slope between the lines, the higher the level of interaction. In the same Figure 4.12, it can also be clearly seen that the interaction plots of carbon content (C wt%) with other factors do not have statistical significance where the change in tensile toughness when it moves from the low level to the high level of df, V_m, and $\dot{\varepsilon}$ are about the same at levels of C wt%.

![Interaction Plots for tensile toughness (fitted means)](image)

**Figure 4.12:** Interaction Plots for tensile toughness (fitted means)

It is also obvious that the interaction graphs of the tensile toughness mean show sufficient interaction between ferrite grain size (d_f) and other factors because the lines are not parallel as well as martensite volume fraction (V_m) and strain rate ($\dot{\varepsilon}$). Another key aspect to recall is that these interaction graphs can be used to assess the main effects and interaction influences, provided that
evaluating significance is determined by looking at the p-values for all interaction effects in the Analysis of Variance and the RSM model regression evaluation as shown in Table 4.5.

### 4.3.2.1 Parametric study

The parametric study was conducted by the RSM model, and the effects of the considered factors on each response are shown in Figure 4.13 to Figure 4.18 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 relates to two considered factors.

![Figure 4.13](image)

**Figure 4.13**: 2D Contour and 3D surface plots for toughness with ferrite grain size (d_f) and martensite volume fraction (V_m)

The 2D contour, Figure 4.13 (b), shows that increases in toughness from the lower range to the higher range V_m is greater at the middle range of d_f and the largest toughness is achieved when d_f values are low, and V_m values are high. This highest toughness range shows at the upper left corner of the plot, which is greater than 240 MJ/m³. The provided graph in Figure 4.13 (a) shows the tensile toughness increases gradually with rising d_f until the mid-level of d_f and then decreases with increasing d_f, while the tensile toughness moderately increases with going up V_m.
Figure 4.14: 2D Contour and 3D surface plots for toughness with carbon content (C wt%) and strain rate (\(\dot{\varepsilon}\)).

As is presented in Figure 4.14 (a), the carbon content in DP steels does not have any statistical significance on toughness, which is clearly confirmed by horizontal lines in the 2D contour plot. A glance at the 3D surface plot, Figure 4.14 (b), reveals that the tensile toughness remains constant with rising C wt% whereas it increases dramatically with rising \(\dot{\varepsilon}\). The 2D contour plot in Figure
4.15 (a) demonstrates the energy absorption capacity increases with going up both $V_m$ and $\dot{\varepsilon}$ and the higher toughness value that is greater than 280 MJ/m³ is at a high level of $V_m$ and $\dot{\varepsilon}$. The 3D surface plot, Figure 4.15 (b), indicates that toughness upsurges as both $V_m$ and $\dot{\varepsilon}$ increase.

![Figure 4.15: 3D surface plot showing energy absorption capacity](image1)

![Figure 4.15: 3D surface plot showing toughness](image2)

Figure 4.16: 2D Contour and 3D surface plots for toughness martensite volume fraction ($V_m$) and carbon content (C wt%).

![Figure 4.16: 2D Contour and 3D surface plots for toughness](image3)

Figure 4.17: 2D Contour and 3D surface plots for toughness with ferrite grain size ($d_f$) and strain rate ($\dot{\varepsilon}$).

![Figure 4.17: 2D Contour and 3D surface plots for toughness](image4)
The 2D contour plot in Figure 4.16 (a) illustrates that the carbon content in DP steels does not have any statistical significance on the energy absorption capacity of DP steels, which is clearly confirmed by vertical lines. In Figure 4.16 (b) tensile toughness remains constant with rising C wt% whereas it rises considerably with increasing V_m. As shown in Figure 4.17 (a), for lower levels of d_f, strain rate (\dot{\varepsilon}) has slightly effect on the tensile toughness; on the other hand, strain rate (\dot{\varepsilon}) has considerable influence on the tensile toughness at higher levels of d_f. in Figure 4.17 (b), There is a plateau at lower levels of d_f and \dot{\varepsilon}.

![Figure 4.18: 2D Contour and 3D surface plots for toughness with ferrite grain size (d_f) and carbon content (C wt%)](image)

As can be seen in the 2D contour plot in Figure 4.18 (a), the toughness climbs slowly as the d_m increases up to about 4 to 5 μm, then it declines. Moreover, the 3D surface plot in Figure 4.18 reveals that maximum toughness is obtained when d_f values are at middle values. This maximum toughness region that is greater than 200 MJ/m3 shows in the middle of the plot. As mentioned before, the vertical lines in 2D contour mean that the influence of C wt% on the energy absorption capacity of DP steels does not have any statistical significance.
A glance at all graphs reveals that the trend of tensile toughness, Figure 4.13 (b), Figure 4.14 (b), Figure 4.15 (b), Figure 4.16 (b), and Figure 4.17 (b), increases with rising $V_m$ and $\dot{\varepsilon}$ while there is a peak (a clear optimum status) at the certain level of $d_f$ (approximately 4 µm). Not to mention, the given Figure 4.14 (a), Figure 4.16 (a) and Figure 4.18 (a) shows a slight steadiness in the tensile toughness with increasing C wt%.

In order to sum up the results in Figures 4.13 to 4.18, Figure 4.19 shows the relationships between the response and the considered factors, which represents response means for each level of factors. The main effect plot shows that the toughness increases significantly with rising $V_m$ and $\dot{\varepsilon}$ while it remains slightly constant with changing C wt%. It may be seen clearly that the energy absorption capacity of DP steels rises moderately with increasing $d_f$, and it reaches its peak at $d_f$ value equals 5 µm and then it drops off.

Through this study that used, for the first time, the comprehensive statistical parametric study, we found that the maximum tensile toughness in Figure 4.13 (a) and (b) at optimum ferrite grain size ($d_f$) increases with martensite volume fraction ($V_m$), which is in a good agreement with the study conducted by Delince’ et al. [66]. Moreover, the energy absorption capacity increases as
martensite volume fraction ($V_m$) rises, which is also in good agreement with the studies conducted by Abid et al. [22] and Paul [113]. To put it another way, the martensite volume fraction ($V_m$) is clearly more considerable influence than the effect of carbon content (C wt%) as result of the direct connection between $V_m$ and C wt% in Eq’s (4.5) and (4.6). Not only it is quite unexpected that the tensile toughness has a relative maximum with changing $d_f$, but it is also different than the expected result that was found in Figures 4.9 and 4.10. There is a good match between the effect of strain rate on the tensile toughness and preexisting studies (e.g. [6,8,11,13,44]).

4.3.2.2 Microstructure properties design for performance optimization

Based on the specific application and localization of a component in the structure of a car, different DP steel grades are selected. The vehicle components are essentially characterized by the various ratio of strength to ductility required for processes of metal forming and ability to the energy absorbing during crash events. The RSM model was conducted as a model for designing the microscopic properties in the direction of different design applications, which is included the crashworthiness, by maximizing the tensile toughness. To accomplishing this requirement, the design various microstructure properties ($d_f$, $V_m$, and C wt%) of DP steels under different strain rates is required to achieve the optimum mechanical properties with the considered ranges and the boundaries imposed by the applications. The RSM model optimizer tool demonstrates how various factors affect the predicted response, tensile toughness of DP steel at certain strain rates. The considered microstructure parameters in the optimizer tool can be modified interactively to find the predicted responses for a specific input factor (or factors) setting of interest. The optimization plots, as shown in Figure 4.20 and 4.21, show the influence of each variable (factor) (columns) on responses (composite desirability (rows)) at each chosen strain rate.
The results, in Figure 4.20, shows that the RSM model computes that tensile toughness at strain rate 100 sec\(^{-1}\) are maximized when all microscopic parameters settings are at \(d_{r} = 2.86\), \(V_{m} = 47\%\), \(C\) wt\% = 0.06\%. Likewise, Figure 4.21 presents the setting of microstructure parameters (\(d_{r} = 4.52\), \(V_{m} = 47\%\), \(C\) wt\% = 0.15\%) at a strain rate of 400 sec\(^{-1}\) satisfies the effective and maximizing responses. The desirability (D) evaluates how the settings optimize a set of overall responses, which has a range of zero to one. Thus, the optimization results show that the composite desirability (0.71671 and 0.92197 for Figure 4.20 and 4.21 respectively) is close to 1 and above 0.5, which indicates that the settings of microstructure parameters achieve satisfactory results for all responses as a whole.

**Figure 4.20:** Optimization chart of microstructure parameters for the maximum tensile toughness of DP steel at strain rate 100 sec\(^{-1}\)
The optimum setting of the martensite volume fraction (47%) that obtained from optimization results is in good agreement with the work of Movahed et al. [101], which exhibits the optimum mechanical behavior in respect of tensile toughness. Not to mention that the combined effect of the martensite volume fraction and the carbon content in DP steels has a significant impact on the energy absorption capacity of DP steels with changing strain rate where the model changes the carbon content till achieving an optimum in all responses at a fixed volume fraction (47%). Figure 4.21 depicts the maximum value of tensile toughness that could be achieved for given microscopic parameters at a strain rate of 400 sec\(^{-1}\) within the collision-related conditions. The small ferrite grain size (d\(_f\)) strengthens the ferrite phase, as well as the overall DP steel behavior. Interestingly, the small amount of carbon content (C wt%) in DP steel with high martensite volume fraction (V\(_m\)) increases slightly, which leads to reduce martensitic carbon content and cause the martensite phase to deform plastically during the deformation of the overall DP steel. To verify these optimization results, the obtained optimum tensile toughness values are compared with the experimental results that conducted by Qin et al. [1] as shown in Figure 4.22.
From this Figure 4.22, it can be seen that the obtained optimum results values are higher than experimental results even though they were under strain rates smaller than the experimental study. This indicates that the energy that was absorbed by the obtained optimum microstructure parameters is higher than the one that was absorbed by experimental microstructure parameters.

**Figure 4.22:** Comparison between the experimental, numerical and numerical optimum tensile toughness values at different strain rates.

4.4 Conclusions

In this study, a new effective methodology that combines a full micro/macro multiscale material modeling with the response surface methodology (RSM) was developed to investigate independently the key factors of the microstructure that affect the overall behavior of DP steels under quasi-static and dynamic strain rates conditions. The methodology was adopted to predict the flow stress of DP steels and study the influence of microstructure properties using a multiscale
material model with an elasto-viscoplastic constitutive model for each phase in the DP steel. To our knowledge, this is the first study to use the response surface methodology (RSM) as a comprehensive statistical tool to examine autonomously the influences of microstructure properties and their interactions on mechanical behavior of DP steels and also to find the optimum microstructure parameters, which proves to be a powerful tool for finding optimum microstructure properties for optimum performance. The following are the remarkable conclusions obtained from this study:

1) Not only did the proposed methodology contributes further understanding to improving the energy absorption capacity of DP steels under quasi-static and dynamic strain rates, but it is also important to optimize the microstructure properties to meet the requirements for auto manufacturers, namely, passenger safety and environmental awareness. In other words, the findings suggest that this study of the microstructure parameters effects at various strain rate conditions could provide a method of optimizing not only the microscopic parameters but also possible collision-related data.

2) This study has clearly shown that the simulation results match the experimental behavior of DP steels in terms of mechanical behavior and mesh sensitivity. Moreover, the comprehensive statistical parametric investigation was utilized for the first time in our results to examine the influences of variations of microstructure parameters and interaction, which reveals that the microscopic parameters and their two-way interactions play a significant role in the mechanical behavior of DP steels, as well as it was shown that for these microstructure parameters, the energy absorption capacity of DP steels would be optimized.
3) It is concluded that as the martensite volume fraction ($V_m$) increases the energy absorption capacity based on martensitic carbon content that is a function in $V_m$ and C wt% in DP steel as shown in the proposed equation (4.5) and (4.6). It has been demonstrated that the virtual tensile test, the multi-scale model presents non-trivial optima in the mechanical properties, which is found at 47% of martensite volume fraction ($V_m$) with changing other factors based on the design requirements and strain rate conditions.

4) Based on the simulation results, it can be concluded that the tensile toughness increases gradually when ferrite grain size ($d_f$) rises, and it reaches its peak and then declines. To understand this peaks phenomenon deeply in toughness, a physically based model with higher-order gradient plasticity theory needs to be implemented to explain and study this behavior and further effectively capture the size effect.

5) To achieve the needs of steel manufacturers and the automobile designers to match the components requirements of DP steels in the automobile industry, the methodology presented in this paper provides a pathway to modify and optimize the setting of microstructure parameters interactively, to produce desirable materials for the intended application as well as towards various design requirements. Therefore, the desirable microscopic parameters of DP steels can be controlled by varying intercritical heat treatment temperatures [23].

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CHAPTER FIVE: SUMMARY AND FUTURE WORK

Acknowledging the importance of investigating the relationship between microstructure properties and mechanical properties of dual phase (DP) steels brings technological benefits, as a result from the study of this relationship, and the need for continuous improvement of advanced material for automotive applications. As presented in previous chapters, DP Steels are used widely and commonly in the automobile industry. This Thesis showed a new methodology to study the relationship between the mechanical properties of DP steel and its microstructure properties, as well as the effects and interaction among the microstructure parameters on the mechanical behavior of DP steels by using a multiscale modeling framework coupling with multivariate statistic technique. This framework includes a mean-field homogenization incremental model and a full micro-macro multiscale material model, and an elasto-viscoplastic constitutive model. This framework can capture changing in the mechanical behavior associated with microstructure details and the macroscopic behavior of the multiphase material, DP steels. In addition, the multivariate statistic technique has been carried out for comprehensive analytical parametric study and optimization by using response surface methodology. Using this methodology, the 3D micromechanical modeling was conducted to simulate the mechanical behavior of DP steels using the 3D representative volume element (3D RVE) and statistical analytical investigation was carried out to study independently the effect and interactively interaction of four microstructure parameters: the ferrite grain size, the martensite grain size, the martensite volume fraction, and the carbon content in DP steel, as well as discovering the effective microstructure properties that produce the best possible mechanical properties of DP steels. The numerical and statistical results exhibited that our methodology is an effective means for studying these parameter influences on a combination of strength and ductility and also to find the optimum microstructure parameters.
Another key conclusion from the statistical analytical investigation to highlight is that the interaction among the microstructure parameters plays a significant role in the mechanical behavior of DP steels, which cannot be estimated by traditional methodology.

Moreover, we developed a full micro-macro multiscale material approach, based on structural FEA model with input from mean-field homogenization incremental model, to investigate mechanical properties of the multiphase material, DP steels under different microstructure parameters and strain rates. The simulation results from the multiscale material approach were then used in the RSM approach that was conducted as a model for optimizing the microscopic parameters in the direction of distinctive design requirements, which is metal forming processes and crashworthiness performance. Validation of this approach showed that the numerical results were in good agreement with experimental data in terms of mechanical behavior and mesh sensitivity, which was conducted using a multiscale material model and an elasto-viscoplastic constitutive equation with isotropic yield criterion. It was shown in this approach that the energy absorption characteristic, ultimate strength, and ductility of DP steels could be optimized within the considered microstructure parameters ranges to improve the performance of metal forming operations and crashworthiness for DP steels, as well as this approach can be valuable way for guiding various design requirements based on material design in automotive industry.

Not only did the developed methodology contribute to further understanding of the microstructure properties of multiphase materials, such as DP steels, control the mechanical properties under quasi-static and dynamic strain rates, but it also shows that it is important to optimize these microstructure properties to meet the components requirements of DP steels in the automobile industry, namely, passenger safety and environmental awareness.
The versatility of this developed methodology allows application of our multiscale material and RSM model to other types of statistical analytical investigations in other multiphase materials such as the effect of grain aspect ratio, the direction of rolling, and density and size of voids on the mechanical properties. As we mentioned in the previous chapters, a physically based model with higher-order gradient plasticity theory has been developing to explain and study peaks phenomenon that appeared in toughness and ductility when changing ferrite grain size, as well as further effectively capture the size effect, which is presented in Appendix A. Through this model in Appendix A, a stress and strain gradient model have been implemented to capture grain size effects. 3D RVEs have been generated by the Digimat-FE software, which takes into account distribution, size, volume fraction and orientation of grains for each phase. The following suggestions for future work could be used to achieve this purpose further:

1) Study the deformation behavior of multiphase materials for wide ranges of strain rates and temperatures, common in the metal forming processes, by using Johnson/Cook strain and temperature sensitive plasticity model.

2) Study and design heterogeneous microstructure (grain gradient) that exhibited the capability to lead to better results than some of its homogeneous microstructure.

3) Study porous material with different porosity size and spatial porosity distribution and investigate statistically and systematically in a damage mechanism in DP steels during uniaxial tension testing and to explain the various void nucleation and growth mechanisms.
APPENDIX A : A Method of Coupling Continuum Dislocation Dynamics to the Continuum Plasticity Finite Element Method “CDD-CPFE”

A design of all metallic components fundamentally depends on a classical continuum plasticity theory, which is size independent and unable to predict these effects. According to Chakravarthy and Curtin [119], the physical length scale that controls the flow stress in metals are not clearly established in the conventional continuum plasticity model. However, geometrically necessary dislocations (GND) have been attributed to the length scale controlling size effect, which occurs when plastic strain gradients exist in a material[120]. According to Taheri-Nassaj and Zbib’s study [121], the size effects in plasticity can also be attributed to dislocations pileup in source-obstacles configurations; which leads to stress-gradient plasticity model in the presence of stress gradients.

In this work, A continuum dislocation dynamic model (CDD) coupled with a continuum plasticity finite element (CPFE) model will be used to investigate the mechanical behavior of multi-phase materials where the shared movement of dislocations under the influence of the interactions between the dislocation cores and the crystal lattice, their mutual interactions, and the externally applied loads cause plastic deformation of polycrystalline materials [121–124]. We have been developing the constitutive model of CDD-CPFE that linked the hardening and plastic shear strain rates to the dislocation velocities and dislocation density evolutions using CDD model and describes this plastic strain using CFFE equation.

We built a classical constitutive framework and examined the validity of using viscoplasticity for describing the plastic strain, and we set the requirements that should be satisfied
In a small-strain plasticity problem, the total strain $\varepsilon$ can be decomposed into elastic and plastic parts:

$$\varepsilon = \varepsilon^e + \varepsilon^p$$  \hspace{1cm} (1)

Isotropic linear elasticity is assumed and the elastic strain tensor $\varepsilon^e$ is related to the Cauchy stress tensor $\sigma$ as follows:

$$\varepsilon^e = M : \sigma \quad \text{or} \quad \sigma = C : \varepsilon^e$$  \hspace{1cm} (2)

where $M$ and $C$ are the fourth-order compliance and stiffness tensors. The evolution of the stress is described by a system of differential equations:

$$\dot{\sigma} = C \dot{\varepsilon}^e$$  \hspace{1cm} (3)

By using the additive decomposition, and solving the elastic strain rate, the stress rate is expressed as:

$$\dot{\sigma} = C (\dot{\varepsilon} - \dot{\varepsilon}^p)$$  \hspace{1cm} (4)

The equation (4) includes both the unknown stress rate $\dot{\sigma}$ and the unknown plastic strain rate $\dot{\varepsilon}^p$, which is described later. A fundamental purpose of phenomenological plasticity models is to duplicate the one-dimensional tension test. To achieve this, a scalar equivalent stress, which is defined in terms of the deviatoric stress tensor, is expressed as:

$$\bar{\sigma} = \sqrt{\frac{3}{2} s_{ij} s_{ij}} , \text{ where } s_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}$$  \hspace{1cm} (5)

and an equivalent plastic strain is expressed as:

$$\bar{\varepsilon}^p = \sqrt{\frac{3}{2} \varepsilon_{ij}^p \varepsilon_{ij}^p}$$

which is defined in terms of the plastic strain tensor, and the equivalent stress is set equal to the critical resolved shear stress, $\tau_{crss}$. 

\[ \bar{\tau}(\sigma) = \left( \frac{\bar{\sigma}}{\sqrt{3}} \right) = \tau_{crss} = \frac{1}{\sqrt{2}} s_{ij} s_{ij} \quad (6) \]

The rate of the plastic strain using tensor is given by the form:

\[ \dot{\varepsilon}^p = \sqrt{\frac{3}{2}} \dot{\varepsilon}^p_{ij} \dot{\varepsilon}^p_{ij} = \hat{\gamma}^p \left[ \frac{s}{2\tau} \right] , \quad \dot{\varepsilon}^p = \hat{\gamma}^p \mathbf{N} \quad (7) \]

\[ \hat{\gamma}^p = \hat{\gamma}_0 \left( \frac{\bar{\tau}}{\tau_{crss}} \right)^{\frac{1}{m}} \quad (8) \]

where \( \mathbf{N} \) is the direction of plastic flow for steel is based on the deviatoric stress and the effective shear stress, \( \hat{\gamma}^p \) is the effective plastic shear strain rate, \( \tau_{crss} \) is the critical resolved shear stress for all slip systems, and \( \hat{\gamma}_0 \) is the reference shear strain rate [122]. The \( \mathbf{N} \) relates the macroscopic flow stress, \( \sigma \), and the resolved shear stress, \( \tau \), and the plastic strain, \( \varepsilon^p \), to the amount of crystallographic slip, \( \bar{\gamma}^p \), as follow

\[ \sigma = \mathbf{N} \tau , \quad \mathbf{N} \cdot d\varepsilon^p = d\bar{\gamma}^p \quad (9) \]

From Eq. (9), the macroscopic work hardening rate relates to the microscopic material parameters by:

\[ \frac{d\sigma}{d\varepsilon^p} = \mathbf{N}^2 \frac{d\tau}{d\bar{\gamma}^p} + \tau \frac{d\mathbf{N}}{d\varepsilon^p} \quad (10) \]

where \( \frac{d\tau}{d\bar{\gamma}^p} \) represents the microscopic hardening rate of the crystalline element. The effect of strain on orientation variation is presented by the second term in Eq. (10) [126]. The effective shear strain rate in continuum scale “the Orowan relation” can be calculate by the following equation [122,123]:

\[ \hat{\gamma}^p = \rho^T_M b \bar{\vartheta}_g \quad (11) \]
where $b$ is the magnitude of the Burgers vector, $\rho_T^M$ is the total mobile dislocation density and $\bar{v}_g$ is the average dislocation glide velocity. Here, the average dislocation glide velocity can be calculated by the following equation\(^{[122,123]}\):

$$\bar{v}_g = v_0 \left( \frac{\bar{\tau}}{\tau_{c rss}} \right)^{\frac{1}{m}} \quad (12)$$

The effective plastic strain is given by this equation:

$$\Delta \varepsilon^p = \left( \frac{\bar{\nu}^p}{\sqrt{3}} \right) \quad (13)$$

$\tau_{c rss}$ is the summation of, (1) $\tau_{0ac}$, takes into account the contribution of the lattice friction and the elements in solid solution; (2) $\tau_h$, the resistance from dislocation hardening arising from interaction between dislocations, it can be determined using the Bailey-Hirsch relation; and (3) $\tau_s$, a size-dependent term \(^{[122,123]}\).

$$\tau_{c rss} = \tau_{0ac} + \tau_h + \tau_s \quad (14)$$

the following expression for the first term in Eq. (8) is:

$$\tau_{0ac} = \tau_0 + \sigma_{alloying} + \Delta \sigma_C \quad (15)$$

Where $\tau_0$ is an internal friction term that can be obtained from simulations or experiments, $\sigma_{alloying}$ is the additional strengthening due to alloying elements in the solid solution \(^{[115]}\):

$$\sigma_{alloying} = 77 + 80\% Mn + 750\% P + 60\% Si + 80\% Cu + 45\% Ni + 60\% Cr$$

$$+ 11\% Mo + 5000N_{ss} \quad (16)$$

The third term, $\Delta \sigma_C$, provides strengthening by precipitation or the carbon in solution, in case of ferrite phase it is \(^{[115]}\):

$$\Delta \sigma^f_C = 5000 \times (\% C_{ss}^f) \quad (17)$$
while for martensite it is \[115\]:

\[
\Delta \sigma_c^m = 3065 \times \%C_{ss}^m - 161
\]  

where \(\%C_{ss}^f\) and \(\%C_{ss}^m\) denote the carbon content (in wt\%) in ferrite (0.022 wt\% at room temperature) and martensite, respectively.

Through the mixture role, the \(\%C_{ss}^m\) can be calculated by following equations \[115\]:

\[
\%C = \%C_{ss}^f \times FVF + \%C_{ss}^m \times MVF
\]

Where \(\%C\) donotes the carbon content (in wt\%) in Dual Phase, \(FVF\) and \(MVF\) denote ferrite volume fraction and martensite volume fraction, respectively.

The dislocation hardening term, e.g. \(\tau_h\), is determined with the Bailey–Hirsch relation \[122,123\]:

\[
\tau_h = ab\mu \sqrt{\rho_{SSD}^T}
\]

where \(\mu\) is the shear modulus, \(\alpha\) is a costant. Finally, \(\rho_{SSD}^T\) is the total statistically stored dislocation density (SSD) in materials, defined as \(\rho_{SSD}^T = (\rho_{M}^T + \rho_{I}^T) + \rho_0^T\), where \(\rho_0^T\) is the initial statistically stored dislocation density (SSD) in materials \((\rho_{0M}^T + \rho_{0I}^T)\), and subscripts M and I denote mobile dislocation density and immobile dislocation density, respectively. Dislocation density evolution laws will be introduced into CDD-CPFE. These laws compose of six mechanisms including (1) multiplication and growth of resident dislocations, as well as the production of new dislocations from Frank–Read sources in the slip system, (2) mutual annihilation of two mobile edge or screw dislocations with opposite signs in the slip system, (3) transition from the mobile type to the immobile type due to interactions between dislocations, (4) the mobilization of immobile dislocations due to the breakup of junctions, dipoles, pinning parts, etc., at critical stress conditions, (5) cross-slip, in which screw dislocation segments on one slip
plane move to another glide plane during plastic deformation, and finally (6) annihilation between mobile and immobile dislocations [121–124].

\[
\dot{\rho}_M^T = \left[ \frac{\rho_M v_g}{\bar{l}_g} \right]_1 - \left[ 2R_c \rho_M^2 v_g \right]_2 - \left[ \frac{\rho_M v_g}{\bar{l}_g} \right]_3 + \left[ \frac{\bar{t}}{\tau_{crss}} \rho_T v_g \right]_4 \\
+ \left[ \frac{\rho_M v_g}{\bar{l}_g} \right]_5 - \left[ 2R_c \rho_M \rho_T v_g \right]_6 
\]

(21)

\[
\dot{\rho}_T = \left[ \frac{\rho_M v_g}{\bar{l}_g} \right]_3 - \left[ \frac{\bar{t}}{\tau_{crss}} \rho_T v_g \right]_4 + \left[ 2R_c \rho_M \rho_T v_g \right]_6 
\]

(22)

**Strain and Stress gradient plasticity contribution**

Geometrically necessary dislocations (GND) have attributed to the length scale controlling size effect, and GND occurs when plastic strain gradients exist in a material. Thus, the density of GNDs is included into the mean free path of moving dislocations, \( \bar{l}_g \) [120–125,127]:

\[
\bar{l}_g = \frac{c^*}{\sqrt{(\rho_{SSD} + \|\rho_{GND}\|)}} 
\]

(23)

where \( c^* \) is a constant and \( \|\rho_{GND}\| \) is the density norm of the GNDs:

\[
\|\rho_{GND}\| = \frac{1}{b} \sqrt{\alpha_{ij} a_{ij}} 
\]

(24)

where \( a_{ij} \) is the Nye’s tensor. The rate form of the Nye's tensor for large deformation is given by Shizawa and Zbib [128]

\[
\dot{\alpha} = curl \left( D^p + W^p \right) 
\]

(25)

where \( D^p \) is the strain rate tensor and \( W^p \) is the plastic spin. Here, we assume small deformation, and that the plastic spin is small, and then Eq (25) will be:

\[
\alpha_{ij} = \epsilon_{jmn} \epsilon_{in,m}^p 
\]

(26)
Moreover, the $\rho_{GND}$ is also described as the minimum density of discrete lattice dislocations that is required to accommodate a given mesoscopic strain gradient [129]:

$$\|\rho_{GND}\| = \frac{1}{b} \nabla \bar{\tau}^p$$  \hspace{1cm} (27)

Stress gradient plasticity model that represents a small scale flow stress of the material is implemented into the CCD-CPFE model by including stress gradient terms in calculating the critical resolved shear stress “the Third term in Eq (14), $\tau_s$” [121–124]:

$$\tau_s = \tau_Y \left[ 1 + \frac{L}{4\bar{\tau}} \nabla \bar{\tau} \right]$$  \hspace{1cm} (28)

where $\tau_Y$ is Hall–Petch stress:

$$\tau_s = \frac{K}{\sqrt{L}} \left[ 1 + \frac{L}{4\bar{\tau}} \nabla \bar{\tau} \right]$$  \hspace{1cm} (29)

$K$ is Hall–Petch constant, $\bar{\tau}$ is the effective stress and $\nabla \bar{\tau}$ is its spatial effective shear stress gradient.

A numerical technique, Finite Difference Method (FDM), will be used to obtain the spatial gradient within a finite element framework at each integration point (IP), and the mathematical definition of gradient in Eq’s (27) & (29) within a finite element framework, based on Figure A.1 is as follows.

$$\nabla \bar{\tau} |_{t+\Delta t} = \left. \frac{\partial \bar{\tau}}{\partial x} \right|_t \hat{i} + \left. \frac{\partial \bar{\tau}}{\partial y} \right|_t \hat{j}$$  \hspace{1cm} (30)

$$\nabla \bar{\tau} |_{t+\Delta t} = \left. \frac{\partial \bar{\tau}^p}{\partial x} \right|_t \hat{i} + \left. \frac{\partial \bar{\tau}^p}{\partial y} \right|_t \hat{j}$$  \hspace{1cm} (31)
The CDD-CPFE model has been implemented in Fortran code (flowchart is presented in Figure A.2) using LS-DYNA/UMAT. After successful development of the UMAT, the CDD-CPFE model will be applied on 3D RVE model of DP steels that is generated by Digimat-MF with specific martensite volume fraction as shown in Figure A.3.

**Elastic predictor:**

In a First phase, we conditionally assume that the material behaves elastically and we calculate a trial stress, \( \sigma^{Tr} \), is the deviatoric part of the stress, \( s \), corresponding to the old stress state \( s \) plus purely elastic stress increments \( \Delta \epsilon \)

\[
\sigma^{Tr} = s + 2\mu \Delta \epsilon \tag{32}
\]

Since the pressure is independent of the plastic flow, its update is the same regardless of whether or not there is plastic flow,

\[
P = P - \left( \lambda + \frac{2}{3} \mu \right) tr(\Delta \epsilon) \tag{33}
\]
Figure A.2: Flow chart of Fortran code (UMAT) for CDD-CPFE model
Figure A.3: LS-DYNA input file for 3D RVE generated by Digimat-MF for DP steel (25% $V_m$, total elements 27000)

The equivalent trial stress is evaluated,

$$\bar{\tau}^{Tr} = \sqrt{\frac{1}{2} \sigma_{ij}^{Tr} \sigma_{ij}^{Tr}}$$ \hspace{1cm} (34)

The gradient of the effective shear stress will calculate by Eq (30)

$$\nabla \bar{\tau} = \frac{\bar{\tau}_{l(1+j)} - \bar{\tau}_{l(j-1)}}{2\Delta x} + \frac{\bar{\tau}_{l(1+j)} - \bar{\tau}_{l(j-1)}}{2\Delta y}$$ \hspace{1cm} (35)

The $\tau_{crss}$ can be computed based on $\rho_0^T_M$ and $\rho_0^T_H$ and if

$$\bar{\tau}^{Tr} \leq \tau_{crss} = \tau_{0ac} + \tau_h + \tau_s$$ \hspace{1cm} (36)

then the response is elastic, and the stress at the end of the time step is

$$\sigma = \sigma^{Tr} + PI$$ \hspace{1cm} (37)
Plastic correction by radial return:

When Eq (35) is not satisfied, it means that there is plastic flow due to the motion and interactions of dislocations, which are responsible for hardening of the material, and the increment in the equivalent plastic strain must be calculated. The closest point of the yield surface to the trial stress lies along the line from the origin to the trial stress, and therefore the final deviatoric stress will be proportional to the trial stress, \( \sigma^{n+1} = \alpha \sigma^{Tr} \). From Eq (8), the \( \Delta \dot{\gamma}^P \) and \( \Delta \bar{\gamma}^P \) can be computed:

\[
\begin{align*}
\Delta \dot{\gamma}^P &= \dot{\gamma}_0 \left( \frac{\bar{t}}{\tau_{crs}} \right)^{\frac{1}{m}} \\
\Delta \bar{\gamma}^P &= \Delta \dot{\gamma}^P \cdot \Delta t \\
\bar{\gamma}^{P+\Delta t} &= \bar{\gamma}^P + \Delta \bar{\gamma}^P
\end{align*}
\]

From Equations (27) and (31) and at plastic state, we can calculate \( \nabla \bar{\gamma} \mid_{t+\Delta t} \) and \( \| \rho_{GND} \| \),

\[
\nabla \bar{\gamma}^P \mid_{t+\Delta t} = \left. \frac{\partial \bar{\gamma}^P}{\partial x} \right|_t i + \left. \frac{\partial \bar{\gamma}^P}{\partial y} \right|_t j , \quad \| \rho_{GND} \| = \frac{1}{b} \nabla \bar{\gamma}^P
\]

From Equation (12) and at plastic state, we can calculate \( \bar{v}_g \),

\[
\bar{v}_g = v_0 \left( \frac{\bar{t}}{\tau_{crs}} \right)^{\frac{1}{m}}
\]

Then, From Equation (23) and at plastic state, we can calculate \( \bar{l}_g \)

\[
\bar{l}_g = \frac{c^*}{\sqrt{(\rho_{SSD}^t + \| \rho_{GND} \|)}}
\]

From Equation (11) and at plastic state, \( \Delta \rho_M^T \),

\[
\Delta \rho_M^T = \frac{\Delta \dot{\gamma}^P}{b \bar{v}_g} , \quad \rho_M^{T+\Delta t} = \rho_M^t + \Delta \rho_M^T
\]

Now, we can compute dislocation density evolution laws, \( \dot{\rho}_{SSD}^T \mid_t \), from Eq’s (21 & 22).

The \( \rho_{SSD}^T \) and \( \rho_l^T \) update is completed by
\[ \rho_{SSD}^{t+\Delta t} = \rho_{SSD}^{t} + \dot{\rho}_{SSD}^{t} \Delta t \]  
(40)

\[ \rho_{i}^{t+\Delta t} = \rho_{0}^{t} + \dot{\rho}_{i}^{t} \Delta t \]  
(41)

The effective plastic strain is given by Eq (13):

\[ \Delta \varepsilon^{p} = \left( \frac{\Delta \dot{\gamma}^{p} \Delta t}{\sqrt{3}} \right) \]  
(42)

Once the increment in equivalent plastic strain is calculated, the proportionality factor \( \alpha \), is calculated and the trial stress is scaled back to the yield surface. The stress update is completed by adding the deviatoric and mean stress, \(-P\).

\[ \alpha = \left( 1 - \frac{3\mu \Delta \varepsilon^{p}}{\sigma^{tr}} \right) \]  
(43)

\[ s = \alpha \sigma^{tr} \]  
(44)

\[ \sigma = s - PI \]  
(45)

\[ \bar{\varepsilon}_{total}^{p} |_{t+\Delta t} = \bar{\varepsilon}_{p}^{t} + \Delta \bar{\varepsilon}^{p} \]  
(46)
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