A new method to generate artificial microstructure of dual phase steel using Teacher-Learner Based Optimization

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MS received 3 July 2018; revised 22 November 2018; accepted 10 December 2018; published online 21 March 2019

Abstract. The dual phase steels are widely used in the manufacturing and automobile industry. The micromechanical analysis of the dual phase steel using microstructure based representative volume elements is the effective methodology for the estimation of its macroscopic properties. The real microstructure of the dual phase steels obtained using different microscopic analysis methods depicts the two main constituents viz. martensite inclusion in the ferrite matrix. The distribution of martensite in ferrite matrix exhibits a number of control parameters to define its characteristics. Generation of the artificial microstructure of dual phase steel based on these controlling parameters is advantageous to get a-priori estimate of the macroscopic properties and behavior. In the present work, a model is proposed for predicting the artificial microstructure of dual phase steel. The volume fraction of martensite and connectivity of the martensite in the ferrite matrix are used as controlling parameters to generate the artificial microstructure using the Teacher-Learner Based Optimization algorithm. The model has effectively predicted the microstructure of the DP590 steel. The artificial microstructure is applied for getting the tensile flow curve of the material using the finite element method. The predicted tensile response of the material is in good agreement with the experimental observations for DP590 steel. The model can be effectively applied to predict the artificial microstructure and subsequent micromechanical analysis of the dual phase steels.

Keywords. Dual-phase steel; artificial microstructure; micromechanical modeling; Teacher-Learner Based Optimization; Finite Element Analysis.

1. Introduction

The lightweight and high strength materials are increasingly used in manufacturing industries. The demand for lightweight vehicles is the need of the hour for fuel economy, crashworthiness, and improved performance. In view of such demands, the steel industry is developing higher strength steels called as advanced high strength steels (AHSS). These AHSS grades have high strength and formability characteristics in comparison to the conventional steels and are easily adaptable to the manufacturing sector. The main constituents of these grades are ferrite and martensite. Dual-phase (DP) steels, transformation-induced plasticity (TRIP) steels, and complex phase (CP) steels are some of the examples of AHSS steels. In these steels, hard phase martensite is located throughout in the soft matrix phase of ferrite. In DP steels, martensite is present either in random order or in the banded form surrounded by the ferrite matrix. It is reported that the DP steels have strength in the order of 400–1000 MPa with elongation in the range

10–30% [1]. The micro-mechanical analysis of the DP steels is performed for predicting the macroscopic elastic–plastic flow behavior. The analytical approaches based on homogenization methodology are used to get the flow curve. Tomota *et al* [2] predicted the macroscopic stress–strain response of multi-phase steels using the stress–strain curves of the physical constituents. They defined a concentration factor which is a function of volume fraction, shape and distribution of grains of the component phases, and strain, etc. They predicted different properties of a number of multi-phase materials for the validity of the methodology. Uppaluri and Gautham [3] predicted the strain hardening curve of DP steels. They used a dislocation-based strain hardening model combined with a Mori-Tanaka homogenization scheme for estimating the effective properties of the DP steel from its constituents. The model was applied to the tensile simulation on ABAQUS. They found that the total plastic deformation was confined to ferrite matrix only.

The alternate approach for predicting the flow curve of dual phase steels is to perform the micromechanical analysis using representative volume element (RVE) and finite

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element method. The RVE is obtained from real microstructure obtained from the microstructural analysis of the material or an artificial microstructure of the DP steel. The real microstructure-based models are created by X-ray and neutron diffraction, scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), etc. Sun *et al* [4, 5] performed the micro-mechanical analysis on the real microstructure obtained from the metallographic image obtained from SEM. They found that the ductility of the dual-phase steels is dependent on the volume fraction of the martensite and the local failure mode and ultimate ductility of dual phase steels are closely related to the stress state in the material driven by the plastic strain localization. Marvi-Mashhadi *et al* [1] used real microstructure obtained from SEM image for finite element (FE) study using ABAQUS. The properties of the constituent phases were obtained from the in-situ measurement. They found a good correlation between the actual and predicted flow curve of DP steel. Ramazani *et al* [6, 7] used a real microstructure obtained from the SEM image for the analysis. They studied the effect of microstructural banding and the effect of grain size on the prediction of flow curve. They found that the equiaxed microstructure shows higher strength and work hardening in comparison to the banded microstructure of DP steel. Ramazani *et al* [8] found that the 2-dimensional (2D) microstructure is computationally efficient but in the actual 3-dimensional (3D) deformation, the 2D approach may not be able to predict the actual material behavior. They observed that efficient 2D microstructure can be generated from the real microstructure but statistical algorithms are used for generating the 3D microstructure. They predicted a correlation for the deformation from 2D to 3D based on the polynomial approximation regarding martensite fraction and equivalent plastic strain. Madej *et al* [9] have used real microstructure obtained from the SEM image and processed it using digital material representation (DMR) concept for getting a robust FE model incorporating the influence of size, shape, and position of the constituent phases. Hosseini-Toudeshky *et al* [10] investigated the pattern of deformation in the microstructure of the dual phase steels. They used micromechanics representative geometry generated on SEM image and the finite element mesh confirming to real shape of grains. They obtained the macroscopic flow behavior incorporating the characteristics of the interface elements between martensite and ferrite. They reported that the elastic–plastic deformation with separate interface elements can predict the void initiation at the martensite boundaries. Sirinakorn [11] used real microstructure and finite element analysis on the RVE to obtain the flow curve of DP steel. They used stress–strain data for ferrite and martensite in addition to transformation induced Geometrically Necessary Dislocations (GNDs) in the RVE for getting the macroscopic response. They found that the martensite triple junctions have the highest stress concentration leading to the crack initiation in the microstructure. Brands *et al* [12] constructed three-

dimensional (3D) RVE from the 3D-EBSD. They used a set of cross-sectional planes extracted via “sequential serial sectioning” for the reconstruction of the 3D RVE. The basic parameters used for reconstruction were phase fraction of martensite and specific internal surface density specifying the fineness of distributed martensite inclusions in a ferrite matrix. They found a large deviation in the results of mechanical experiments using the discretization of the 3D structures. They proposed a “statistically similar volume elements (SSVEs)” for improving the mechanical results.

The micromechanical analysis using artificial microstructure is alternatively used for predicting the macroscopic properties of dual phase steels. In one of the simplifications, the statistical description is used to generate the artificial microstructure. In few of the works, geometrical primitives viz. spheres, polygons or polyhedral are used for generating artificial microstructure. Al-Abbasi and Nemes [13, 14] performed micromechanical analysis assuming spherical martensitic particles dispersed in a soft ferritic matrix as a representative microstructure for DP steels. They also studied square and hexagonal approximations of the martensite phases in a ferrite matrix. They observed that the effect of changes in the macroscopic properties can be captured with a hexagonal microstructural approximation. Lai *et al* [15] used hexagonal packed artificial microstructure to find the effect of volume fraction of martensite and its hardness on tensile behavior of the DP steel. They found that the hardness of the martensite phase has minimal effect on the flow curve variation.

The microstructure generated using geometrical primitives assumes a number of approximations. The Voronoi cells in the Voronoi tessellation [16] are random in size and the distribution is generated from random seed points in a defined domain. Due to the randomness of the distribution, size, and shape of the cells, Voronoi tessellation is effectively used for generating artificial microstructure of DP steels. Abid *et al* [17] proposed a model to generate the artificial microstructure. They used an optimization and filtering algorithm along with post-Voronoi treatment to resemble the microstructure of the DP steel. They used a uniform random distribution of seeds for the Voronoi tessellation to get an equiaxed microstructure. They showed that such artificial microstructure is able to capture the realistic microstructure and can be used effectively for the prediction of macroscopic flow curve of DP steels. Vazragupta *et al* [18] used a multiplicatively weighted Voronoi tessellation (MW-Voronoi) algorithm to generate the artificial microstructure geometry model. They used average grain size and the grain size distribution function describing the microstructure as input parameters for the model. They found that the artificial microstructure obtained using gamma distribution applied to MW-Voronoi is in better agreement than the log-normal distribution. Fillafer *et al* [19] used the Voronoi-tessellation and a proper “coloring” scheme for modeling. The volume fraction of martensite

phase and the contiguity of martensite were used as control parameters for microstructure generation. They employed a “soft” criterion for selecting the appropriate Voronoi-cell as martensite phase and remaining are considered as a part of ferrite matrix. Hou *et al* [20] used modified Voronoi-tessellation for generating microstructure. They used material Topology Optimization methodology [21] for the phase assignment. The Topological optimization methodology [21] uses a gradient-based algorithm for getting the optimum solution. They found that microstructure generated using Voronoi-tessellation obtained from the uniform random sequence (Pseudo-Random) underestimates the flow curve whereas the Voronoi-cells obtained using Halton sequence (Quasi-Random) are regular in shape and give a convergent solution for the microstructure.

In the present work, an attempt is made to generate the artificial microstructure of the dual phase steel using Voronoi tessellation, the control parameters viz. volume fraction and connectivity of the martensite which are used for defining the microstructure and operated with a population-based Teacher-Learner Based Optimization (TLBO) algorithm proposed by Rao [22]. The optimization algorithm had been applied to a number of constrained and un-constrained engineering design problems [22]. The input to this optimization algorithm requires population size, elite size and convergence criterion. Further, there are no other algorithm-specific parameters for the TLBO methodology [22]. The model is applied to generate the artificial microstructure of DP590 steel [23] and thereafter prediction of macroscopic properties. Subsequently, the developed model is applied to find the effect of different control parameters on the microstructure and the resulting effect on macroscopic properties of dual phase steel.

2. Teacher-learner based optimization (TLBO) algorithm

A number of optimization algorithms are available for solving engineering problems. Rao [22] proposed Teaching–Learning-based optimization (TLBO) algorithm. The elite based TLBO methodology replaces the worst solution by the elite solution during each of the generations. The available evolutionary based optimization algorithms require the input parameters viz. population size, elite size, and convergence criterion, etc. In addition, there are few algorithm-specific parameters which need to be controlled for getting the acceptable optimized solution. The TLBO algorithm requires only the input parameters and does not require any algorithm-specific parameters [24]. The salient points of the algorithm are presented in brief. The details of the formulation and implementation procedure of the algorithm are given in Rao [22].

A population of solutions is assumed as an initial condition to achieve an optimal solution. The assumed

population is a group of “Teachers” teaching a class and a group of “Learners” in a class. The “Learners” are offered different subjects by the different “Teachers” and the result of these “Learners” is treated as a “fitness” function. The teacher is considered as the best solution obtained so far. The TLBO algorithm is divided into two main stages; “Teacher Phase” and “Learner Phase”. In the “Teacher Phase,” the learners learn from the teachers. As per formulation, a teacher tries to improve the result of the class in the subject which the “Teacher” is teaching. The improvement in the result is measured by the increase in the mean result of the class in the subject. The updated solution after the “Teacher Phase” is given by

$$X'_{j,l,i} = X_{j,l,i} + r_i(X_{j,l,best,i} - T_F M_{ji}) \quad (1)$$

where index “*i*” is for iteration, “*j*” for the subject and “*l*” is for “Learner”, $X'_{j,l,i}$ is the updated value of $X_{j,l,i}$, $X_{j,l,best,i}$ is the result of the best learner in the j^{th} subject and in i^{th} iteration, M_{ji} is the mean result of the learner. The “Teaching Factor”, T_F , decides the value of mean to be changed, and r_i is the random number in the range (0, 1). Further, “Teaching Factor” is not an algorithm specific parameter of the TLBO algorithm and can be either 1 or 2, selected randomly with equal probability. All the accepted function values at the end of the “Teacher Phase” are maintained and these values become input to the “Learner Phase”. The “Learner Phase” is the second part of the algorithm where the “Learners” improve their knowledge by mutual interaction among themselves. A learner is imagined interacting randomly with other learners. Let “P” and “Q” are the two learners randomly selected such that $X'_{total-P,i} \neq X'_{total-Q,i}$ (where $X'_{total-P,i}$ and $X'_{total-Q,i}$ are the updated functional values of “P” and “Q”, respectively, at the end of “Teacher Phase”). The updated solution after the “Learner Phase” is given by

$$X''_{j,p,i} = X'_{j,p,i} + \text{abs}\left(r_i(X'_{j,p,i} - X'_{j,q,i})\right) \quad (2)$$

$X''_{j,p,i}$ is accepted, if it gives a better functional value [22]. The detailed flow chart for the elitist-TLBO algorithm [22] is represented in figure 1.

3. Finite element formulation

The finite element equations are developed based on equilibrium equations [25]. For large deformation problems, involving plastic deformation, the updated Lagrangian formulations is used. The details of the mathematical formulation are given in Saxena and Dixit [26]. Some of the important highlights of the formulation are given as follows.

The incremental logarithmic strain measure, used in the present formulation is defined by

$${}^t\Delta\epsilon_{ij}^L = \ln({}^t\ell_i)\delta_{ij} \quad (\text{no sum over } i) \quad (3)$$

Figure 1. Flow chart for elitist-TLBO algorithm [22].

where δ_{ij} is the Kronecker's delta and ${}^t\ell_i$ are the principal values (corresponding principal axis directions are used for stress updation to maintain the objectivity of the stress in large deformation problems) of the incremental right stretch tensor [26].

The incremental elastic–plastic, stress–strain relationship is expressed as

$${}_t\Delta\sigma_{ij} = C_{ijkl}^{EP} \Delta e_{kl}^L \quad (4)$$

The tensor ${}^tC_{ijkl}^{EP}$ is the fourth order elastic–plastic constitutive tensor. Radial backward return algorithm is used for iterative calculation of the incremental stress tensor in Eq. (4).

The integral form of the equilibrium equation at a time $t + \Delta t$ is given by the following virtual work expression [25]:

$$\int_{t+\Delta t V} {}^{t+\Delta t}\sigma_{ij} \delta({}^{t+\Delta t}\epsilon_{ij}) d{}^{t+\Delta t}V = {}^{t+\Delta t}R \quad (5)$$

Here, ${}^{t+\Delta t}V$ is the domain, ${}^{t+\Delta t}R$ is the virtual work of the external forces and ${}^{t+\Delta t}\sigma_{ij}$ the Cauchy stress tensor, all at the time $t + \Delta t$. Further, $\delta({}^{t+\Delta t}\epsilon_{ij})$ represents the virtual linear strain tensor corresponding to the virtual displacement vector $\delta^t u_i$ at time. After suitable modifications and approximations [26], the equation is denoted as

$$\begin{aligned}
& \int_V {}^t C_{ijkl}^{EP} \Delta \varepsilon_{kl} \delta({}_t \Delta \varepsilon_{ij}) d^t V + \int_V {}^t \sigma_{ij} \delta({}_t \Delta \eta_{ij}) d^t V \\
& + \int_V {}^t \sigma_{ij} \delta({}_t \Delta \varepsilon_{ij}) d^t V \\
& = {}^t R
\end{aligned} \quad (6)$$

where the tensors ${}_t \Delta \varepsilon_{ij}$ and ${}_t \Delta \eta_{ij}$ are the linear and non-linear part of the Green-Lagrangian strain tensor [25]. The finite element equations are developed from Eq. (6) [26] after substitution of elemental representation in terms of shape function for the assumed finite element and the assembly over all the elements, leads to the following algebraic equation:

$${}^t [K] {}^t \{\Delta u\} + {}^t \{f\} = \{F\} \quad (7)$$

Here, ${}^t \{\Delta u\}$ is called as the global (incremental) displacement vector and ${}^t [K]$ is the global coefficient matrix, ${}^t \{f\}$ is global internal force vector and $\{F\}$ is global internal force vector. The solution of Eq. (7) represents only an approximate solution to the governing equations, because of the linearization and approximation [26]. To minimize the error of the approximating solution, the modified Newton-Raphson algorithm [25] is used.

4. Artificial microstructure generation model

The microstructure of the DP steel consists of martensite and ferrite matrix. Martensite is assumed to be arranged as hard inclusions in the softer ferrite matrix. The mechanical properties of the DP steel are reported to be dependent on the composition, microstructure and the initial austenite phase before required heat treatment [27]. The microstructural parameters which are generally used to characterize the microstructure of the dual phase steels are martensite/ferrite grain size and shape, mean free distance, aspect ratio, banding index, contiguity, and connectivity, etc. [28]. Further, the volume fraction of martensite in the dual phase steel distinguishes its properties and application. The arrangement of the martensite inclusions in the ferrite matrix is characterized by some or all of these microstructural parameters. It is found that the Voronoi-tessellation can effectively imitate the randomness of the grain size and shape in a microstructure. Further, it is reported that the connectivity of the martensite within the ferrite matrix in a dual phase steel is an important parameter for determination of the tensile behavior [29]. The continuous network improves the area of contact between ferrite (soft matrix) and martensite and thereby, results in improvement in the tensile properties of dual phase steels [29]. In view of the above, the volume fraction of martensite and the connectivity of martensite as the microstructural parameters are used to characterize the microstructure of the dual phase steel in the present work.

The connectivity of the martensite in dual phase steel is defined as [30]:

$$\phi = \frac{\phi_{FM}}{\phi_{FM} + \phi_{FF}} \quad (8)$$

where ϕ_{FM} is the number of ferrite/martensite boundaries per unit length and ϕ_{FF} is the number of ferrite/ferrite boundaries per unit length (excluding martensite boundaries). Sarwar *et al* [29] had investigated the effect of connectivity of the martensite on the tensile strength of the dual phase steel. They found that the continuous martensite structure i.e., a higher value of the connectivity of martensite results into a better tensile strength. The other parameter is the volume fraction of martensite in the ferrite matrix. The volume fraction of the martensite is given by the following relationship:

$$\Omega = \frac{\text{Total area of the martensite grains}}{\text{Total domain area}} = \frac{a^T \rho}{a^T I} \quad (9)$$

where, Ω is the volume fraction of the martensite, a is a vector containing the area of each of the cells in a Voronoi diagram, ρ is a vector containing the values assigned to ferrite and martensite islands/grain/cells, respectively within the range (0,1) with '0' for the ferrite and '1' for the martensite cells and I is the identity vector. The multi-objective evolutionary algorithms used for generating such microstructures may have conflicting objective functions. In such cases, the k-optimality approach is a preferred choice over the Pareto optimality condition [31]. In the present work, the objective function for generating artificial microstructure is assumed as an unconstrained problem with both parameters/functions be satisfied simultaneously stated as minimization type.

The objective function of the optimization problem is formulated as:

$$\min f = c_1 * \text{abs}(\Omega - \Omega_{\text{target}}) + c_2 * \text{abs}(\phi - \phi_{\text{target}}) \quad (10)$$

subjected to

$$\begin{aligned}
\rho &= \begin{cases} 0 & \text{for } \Omega_F \\ 1 & \text{for } \Omega_M \end{cases} \\
\forall \rho &\in (0, 1)
\end{aligned} \quad (11)$$

where, c_1 and c_2 are the weight fractions, Ω_F is the area/volume element assigned for ferrite grain, Ω_M is the area/volume element assigned for martensite grains, Ω_{target} is the targeted volume fraction of martensite in the domain, and ϕ_{target} is the targeted martensite connectivity. Further, following constraint is also maintained:

$$\begin{aligned}
\Omega_F \cap \Omega_M &= \emptyset, \text{ and} \\
\Omega_F \cup \Omega_M &= \Omega_T
\end{aligned} \quad (12)$$

where $\emptyset$ is the null area/volume and Ω_T is the total area/volume of the domain selected for the generation of the artificial microstructure.

The Voronoi-tessellation is applied to generate the artificial microstructure. The number of seed points in the domain is decided based on the number of desired Voronoi-Cells. These seed points are generated based on the uniform random number generator sequence using inbuilt MATLAB function [32] and the Voronoi diagram is generated using these seed points. Subsequently, the data obtained from this preprocessing step is input to the TLBO optimization function. The optimized microstructure is generated when the termination criterion of the optimization algorithm is satisfied. The microstructure so obtained is converted into a binarized image using inbuilt MATLAB function [33]. This binarized image imitates the microstructure and is used to create the representative volume element (RVE). Later, this RVE is used to generate finite element mesh for subsequent FE analysis for predicting the flow behavior using the homogenization methodology [9].

5. Results and discussion

5.1 Generation of the microstructure of DP590 steel

The model is applied to generate the microstructure of DP590 steel [23]. The chemical composition of DP590 steel is given in table 1. The SEM micrograph of the DP590 steel is given in figure 2. It is observed in the SEM micrographs that there are some lighter gray spots which represent the martensite grains and dark gray large sized zone depicts the ferrite grain in the SEM micrograph. In that way, the small grains of martensite are embedded in the ferrite matrix. The volume fraction of martensite inclusions is 10% with remaining ferrite matrix in DP590 steel. There is a number of methods to find the connectivity of the martensite [34–36]. In the present work, hit and trial approach is applied to find the connectivity of the martensite using the correlation of artificial microstructure and the SEM image of the DP590 steel as RVE for the finite element analysis. The connectivity of the martensite is found to be 0.20 after the detailed analysis of SEM micrograph viz-a-viz artificial microstructure.

The artificial microstructure is generated using Voronoi-tessellation. A total of 1000 random seed points is selected for the generation of Voronoi diagram. But the algorithm is not dependent on the number of seed points, which is detailed in the later part of the section. Further, the too low value of number of seed points is not able to capture the actual morphology of the microstructure and too high value

increases the computational cost. The random seed points are generated using the in-built uniform random number generator (Pseudo-Random generator) using MATLAB. Figure 3 shows the Voronoi diagram generated with 1000 randomly distributed seed points. The area and edge lengths of each Voronoi cell are used as input to the TLBO optimization algorithm.

The optimization model is applied for the generation of the microstructure of DP590 steel. The class strength of 200 students is selected as the initialization parameter of TLBO algorithm. The number of subjects or the number of variables is the number of Voronoi cells. The model developed based on TLBO methodology is applied for simulation with the termination criterion that both the objective functions are satisfied, respectively. The convergence tolerance of 1×10^{-4} is assumed for the convergence. The artificial microstructure obtained using the TLBO algorithm after converted into the binarized form [33] is shown in figure 4. The white spots represent the martensite in the ferrite matrix represented as black in the developed artificial microstructure shown in figure 4. It is observed that the dispersion of the martensite islands within the ferrite matrix in the developed artificial microstructure is in good consonance to the real microstructure (figure 2) and both the microstructure in reasonable agreement for the present set of the randomization involved. The artificial microstructure is applied for getting the flow characteristics of the DP590 steel.

5.2 Validation of the model

The artificial micrograph obtained in figure 4 is discretized using iso-parametric mesh. It is reported that the size of RVE has a significant influence on the results for simulating macroscopic tensile flow curve for dual phase steels [6]. The size of RVE should be sufficiently large so that it represents all microstructural features and be sufficiently small to represent statistical homogeneity. The minimum acceptable size of RVE for the computational simulation of the equiaxed microstructure of dual phase steel is found to be at least $25 \mu\text{m}$ [6] with at least 19 martensite islands in the ferrite matrix. Further, the effect of mesh size in the range $0.1 \mu\text{m}$ to $2 \mu\text{m}$ is investigated by Ramazani *et al* [7]. It is found that the element length smaller than $0.25 \mu\text{m}$ have a negligible effect on the tensile properties obtained from the micro-mechanical analysis. The representative volume element (RVE) in figure 4 is discretized using hexahedral elements with element length of $0.2 \mu\text{m}$ in the plane of the micrograph with $1 \mu\text{m}$ along the thickness

Table 1. Composition of DP 590 steel, in weight percent [23].

Steel	C	Si	Mn	Al	P	S	Cu	Cr	N
DP 590	0.09	0.35	0.89	0.04	0.015	0.008	0.025	0.022	0.0054

Figure 2. Microstructure of DP-590 steel obtained from SEM [23].

Figure 3. Voronoi-diagram with 1000 seed points.

Figure 4. Artificial microstructure of DP590 steel from present work.

direction. Only one element is taken along the thickness directions. A total of 33750 finite elements are used for simulating the microstructure of the dual phase steel. The RVE is assumed to deform only in the plane and all the out-of-plane degree of freedom (DOF) for all the nodes are fixed. The discretized finite element mesh of RVE for microstructural analysis is shown in figure 5.

The constitutive relationship for the constituent phases of dual phases steel is required for the micromechanical finite element analysis. The finite element analysis is performed assuming von-Mises yield criterion for the elastic–plastic

Figure 5. Finite element mesh for microstructural simulation.

analysis, associative flow rule, and the isotropic hardening for each of the phase viz. ferrite and martensite. Many researchers have studied the mechanical behavior of these constituent phases of DP steels using different methods namely, nano-hardness or ultra-microhardness [37, 38], in-situ neutron diffraction [39], in-situ high-energy X-ray diffraction techniques [40–42] or micropillar compression method [43–46]. The isotropic hardening behavior of each constituent phase is defined using the dislocation-based model [47–49]. The unified stress–strain relationship for ferrite and martensite is given by [50, 51]

$$\sigma = \sigma_y + \alpha MG \sqrt{b} \sqrt{\frac{1 - \exp(-MK_r \varepsilon)}{K_r L}} \quad (13)$$

where σ is the flow stress at true strain ε and σ_y is the yield stress of the respective constituent phase. The other variables in the relationship are defined in table 2.

The tensile flow curves for ferrite and martensite phases of DP590 steel using Eq. (13) and the data from table 2 are given in figure 6. The flow behavior of these individual phases is incorporated to predict the macroscopic flow curve of DP590 steel using micromechanical analysis. The periodic boundary conditions [52] are applied for the microstructural analysis using the finite element analysis. The periodic grain fragments that intersect the surfaces of RVE are assumed as a single grain to maintain the periodicity of the microstructure. The presented finite element formulation, developed on MATLAB platform for the non-linear large deformation elastic–plastic analysis [26], is applied for the microstructural analysis of RVE. The finite element mesh detailed in the previous section is used for the analysis.

The predicted flow curve obtained from the finite element analysis of the RVE generated using the artificial micrograph is given in figure 7. The homogenization methodology [9] is adopted to obtain the macroscopic response of the dual phase steel. For the comparison purpose, the experimental flow curve of DP590 steel [23] is also plotted in figure 7. It is observed that the predicted tensile stress–strain curve of the macroscale for DP590 steel is in reasonable agreement with the experimental record for the steel [23].

Table 2. Constants for the unified stress–strain relationship [23].

Name of constant	Value
A constant (α)	0.33
Taylor factor (M)	3
Shear Modulus (G)	80 GPa
Burger's vector (b)	2.5×10^{-10} m
Recovery rate (K_r)	1.1: for ferrite 41: for martensite
Dislocation mean free path (L)	5×10^{-6} : for ferrite 3.8×10^{-8} : for martensite

Figure 6. True stress and True strain relationship for ferrite and martensite in DP590 steel [23].

The analysis for the distribution of plastic strain in the microstructure is also investigated. The analysis is performed with the artificial microstructure given in figure 4 and the SEM based microstructure given in figure 2. The other analysis parameters and the finite element mesh for both the microstructure are kept the same. The pattern of equivalent plastic strain in both the cases is given in figure 8. It is observed that the pattern of equivalent plastic strain obtained from both the analysis is in good agreement. These results establish that the proposed model is able to capture the deformation pattern of the dual phase steel to reasonably acceptable values and the model is able to effectively predict the flow behavior of the dual phase steel. Now, the model is applied to study the effect of various controlling parameters on the microstructure and subsequently the prediction of resulting flow curve of the dual phase steel.

5.3 Effect of the volume fraction of martensite

The volume fraction is the prominent factor determining the composition of martensite in the ferrite matrix. The martensite being the harder material with respect to ferrite;

Figure 7. True stress and True strain curve of DP590 steel.

dominates the overall response of the material if it is present in a higher percentage.

The artificial microstructure of DP590 steel is generated with the volume fraction of 15%. The number of seeds for the Voronoi diagram is 1000 and generated using the uniform random number generator. The connectivity of martensite is kept at 0.20 for the analysis in this case. The class strength for the TLBO algorithm is kept at 200 and there is no other controlling parameter for the optimization algorithm. The predicted artificial microstructure of DP590 steel with 15% volume fraction of martensite and with the connectivity of martensite equals 0.20 is given in figure 9(b). It is observed that the martensite is more in distributed form with finer or smaller particles/grains in the ferrite matrix at some places and at other places long connected martensite particles in comparison to the similar artificial microstructure obtained with 10% volume fraction of martensite (figure 9). The connectivity of martensite in both the predicted microstructure is same and due to this fact, the martensite grains are found to be more uniformly distributed with finer/smaller grains at some places and at other places more of the connected martensite particles in the predicted microstructure.

The generated artificial microstructure is applied for the prediction of True stress and True strain response of DP590 steel having 15% volume fraction of martensite. The number and element size is kept the same as discussed before. The finite element mesh is subjected to the periodic boundary condition. The flow curve characteristics of ferrite and martensite are given in figure 6. The comparison of characteristics of flow curve with the varying volume fraction of martensite is shown in figure 10. The response is as expected due to the fact that the flow curve of dual phase steel is found to be dominated by martensite with higher martensite content. Therefore, the tensile response of DP590 steel with 15% volume fraction of martensite is

Figure 8. Equivalent plastic strain distribution during analysis with artificial microstructure and real microstructure.

Figure 9. Effect of volume fraction on the microstructure.

steeper in comparison to 10% volume content of martensite for the similar flow curve behavior.

5.4 Effect of connectivity of martensite

The other important controlling parameter is connectivity of the martensite (ϕ) in the dual phase steel. The connectivity of the martensite is defined by Eq. (8). The model is applied to generate the microstructure with the different connectivity of martensite. The volume fraction of the martensite is kept at 10% and the number of seed points to generate the Voronoi-diagram is 1000. Further, the class strength of the TLBO algorithm is assumed to be again 200. The predicted microstructure with varying values of connectivity of martensite is shown in figure 11. It is observed that the martensite particles are very fine with $\phi = 0.32$ in comparison to the microstructure obtained with $\phi = 0.20$. The higher value of connectivity of martensite keeping the same volume fraction disperses the martensite in the ferrite matrix with finer particles. The fine martensite particle with the higher connectivity of martensite and the same value of

Figure 10. Effect of the volume fraction of martensite on the flow curve.

volume fraction of martensite is in conformation to the fact that the higher value of ϕ results in a higher ratio of a number of interactions between martensite and ferrite.

Figure 11. Effect of connectivity on the microstructure.

The microstructure obtained using the different values of connectivity of martensite is applied for the flow curve determination of DP590 steel. The mechanical properties of ferrite and martensite and other conditions of the analysis are same as discussed in the previous sections. The flow characteristics of DP590 steel with varying values of connectivity of martensite is shown in figure 12. It is observed that the higher value of connectivity of martensite results into the strengthening of the flow properties of the DP590 steel. It is reported that the connectivity of martensite affects the interfacial area between the martensite particles and ferrite [53, 54]. The increase in the interfacial area assists in the stress transfer during tensile deformation of the DP steel [29, 30]. Therefore, the increase in the connectivity of martensite results into increase in the tensile properties of DP590 steel.

Figure 12. Effect of connectivity of martensite on the flow curve.

5.5 Effect of number of random seed points

The Voronoi diagram is generated from the random seed points defined in the domain. The number of seed points affects the size, shape, and distribution of the Voronoi cells in the diagram. A study is performed to find the effect of a number of such seed points on the microstructure and the resulting flow stress of DP590 steel. The seed points are varied for 1000 and 2000. The resulting Voronoi diagram for both the cases is shown in figure 13. There is a clear difference in the size, shape, density, and distribution of the Voronoi cells. It is observed from figure 13(b) that the size of individual Voronoi cells is much smaller in comparison to the same generated with 1000 random seed points. When the number of seed points are more, then there are more number of cells which constitute the individual martensite particles in the ferrite matrix. Further, in view of the present formulation, the more number of smaller sized cells within the same domain results into more number of edges in total which is interacting with the respective adjoining cells.

The Voronoi diagram with a different number of seed points is used for getting the artificial microstructure. The predicted microstructure with a different number of random seed points is given in figure 14. It is observed that the number of random seed points affects the size of individual martensite particles. The martensite particles are more uniformly but randomly dispersed with a greater number of random seed points.

The predicted microstructure obtained using a different number of seed points is used for micromechanical analysis. The analysis details are discussed in the previous sections. The predicted stress–strain response of the artificial microstructure with a different number of random seed points is given in figure 15. It is observed that the number of random seed points used for generating Voronoi diagram and the resulting microstructure has a negligible effect on the predicted stress–strain response of DP590 steel.

Figure 13. Voronoi diagram for the different number of seed points.

Figure 14. Effect of number of seed points on the microstructure.

5.6 Effect of random number generator algorithm

The proposed algorithm for generating artificial microstructure of the dual phase steel is checked for the algorithm and sequence of random number generators for checking the effectiveness of predicted flow curve of the DP590 steel. For the computational purpose, two different methods of random number sequence viz. Pseudo-Random (PR) and Quasi-Random (QR) sequences are widely used. A Pseudo-Random number generator generates a random number based on an initial value or state and has good statistical properties. The initial value could be some random number but the same initial value/state always reproduces the same random sequence. The Quasi-Random number generator generates the random number with a high level of uniformity in a multidimensional space. In a two-dimensional space, the QR numbers cover the domain evenly producing a regular grid [55].

Figure 15. Effect of number of seed points on the flow curve.

Figure 16. Voronoi diagram for different random generator algorithms.

The Voronoi diagrams generated using Pseudo-Random numbers and Quasi-Random sequence are given in figure 16. The total of 1000 seed points is used respectively for generating both the Voronoi diagram. It is observed that the distribution of Voronoi cells in terms of size, shape, density, and distribution is uniform with Quasi-Random sequence whereas the cells are statistically distributed with a Pseudo-Random sequence. The martensite particles in the dual phase steel are arbitrary shaped and randomly placed in the domain. It is assumed that the shape of the cell should not have any effect on the macroscopic prediction of the stress–strain response of DP steel. The Voronoi diagram generated from both the random number generators are applied for predicting the artificial microstructure using the proposed formulation. The volume fraction and connectivity of martensite are 10% and 0.20, respectively. The predicted microstructure using both the random number generator algorithms are given in figure 17. It is observed that the martensite particles are evenly distributed in both

cases. The size of the martensite particles is fine with QR sequence whereas the PR sequence gives comparatively large-sized martensite particles due to the fact that the range of size of Voronoi cells is large with PR sequence and it is more uniform with QR sequence. The connectivity of martensite depends on the number of interactions between martensite and ferrite whereas, the total volume fraction of the martensite depends on the size of the individual Voronoi cells in the domain.

The predicted microstructure is applied for getting the macroscopic True stress and True strain response of DP590 steel. The detailed procedure for the finite element analysis is already discussed in the previous sections. The stress–strain response of DP590 steel using artificial microstructure generated with both the random number generator algorithms are given in figure 18. It is observed that there is the negligible effect of the random number generator algorithm on the predicted macroscopic response obtained from the artificial microstructure generated using the

Figure 17. Effect of random number generator on the microstructure.

Figure 18. Effect of random number generator on the flow curve.

proposed methodology. The volume fraction of martensite and connectivity of the martensite is same for generating the artificial microstructure using both the algorithms, therefore, the proposed formulation is able to generate the artificial microstructure which is independent of the random number generator algorithm.

The Pseudo-Random sequence is based on a deterministic random generator algorithm and the values of the subsequent random numbers are dependent on the initial value or state. The different initial value or state gives an entirely different random number sequence. The seed points used for generating the Voronoi diagram are these initial random numbers generated with a particular value of the state for the Pseudo-random sequence. Further, the different seed points in the given domain generate entirely different Voronoi diagram in terms of size, shape, density, and distribution of the cells. Therefore, a study is performed

to find the effect of initial value or state on the predicted macroscopic tensile response. The Voronoi diagrams generated using two different random initial values are given in figure 19. The total number of 1000 seed points are used respectively for generating both the Voronoi diagrams. The initial value used for generating Voronoi diagrams in figures 19(a) and 19(b) are entirely different. The difference in the size, shape, density, and distribution of the Voronoi cells is clearly visible from figures 19(a) and 19(b), respectively.

These different Voronoi diagrams given in figures 19(a) and 19(b) are applied for generating the artificial microstructure using the proposed formulation. The assumed values of volume fraction and connectivity of martensite are 10% and 0.20, respectively. The predicted microstructures are given in figures 20(a) and 20(b), respectively. It is observed that there is a clear difference in the distribution of martensite particles and different sized martensite particles are randomly distributed in the ferrite matrix. The martensite particles of different size and shape are statistically placed in the domain.

The predicted microstructure is applied for getting the macroscopic True stress and True strain response of DP590 steel. The detailed procedure for the finite element analysis is already discussed in the previous sections. It is found that there is a negligible effect on the predicted flow curve due to the difference in the Voronoi diagram generated with a different initial value for the Pseudo-Random generator. The result of the flow curve is in-line with the response predicted in figure 18 and therefore it is not presented here. The assumed value of volume fraction of martensite and connectivity of the martensite is same for generating the artificial microstructure in both the cases of Voronoi-diagram, therefore, the proposed formulation is able to generate the artificial microstructure which is independent of the initial value of the Pseudo-random sequence for generating the Voronoi diagram.

Figure 19. Voronoi diagram for with Pseudo-random sequence with different state.

Figure 20. Effect of the different initial value of a Pseudo-Random sequence on the microstructure.

Figure 21. Effect of different random sequence with the same Voronoi diagram on the microstructure.

The Teacher-Learner based optimization algorithm is discussed in the previous section. The algorithm uses the class-size and the number of variables viz. a number of Voronoi cells as the input parameters for the optimization. The algorithm uses different random numbers to evaluate the fitness function for getting the optimum solution of the objective function. The default random number sequence in MATLAB is based on the Pseudo-Random number generator. It is already stated that the Pseudo-Random algorithm depends on the initial value or state specified. Now, the proposed model is applied to find the effect of different random sequence in TLBO algorithm on the predicted stress-strain response in DP590 steel using the generated artificial microstructure. The Voronoi diagram is generated using 1000 seed points with the same initial value of the Pseudo-Random sequence. The assumed values of volume fraction and connectivity of martensite are 10% and 0.20, respectively. The predicted microstructures with the different random sequence for the TLBO algorithm are given in figures 21(a) and 21(b), respectively. It is observed that

there is a clear difference in the distribution of martensite particles and different sized martensite particles are randomly distributed in the ferrite matrix. The martensite particles of different size and shape are statistically placed in the domain.

The predicted microstructure is applied for getting the macroscopic True stress and True strain response of DP590 steel. The detailed procedure for the finite element analysis is already discussed in the previous sections. It is found that there is a negligible effect on the predicted flow curve due to the difference in a random sequence for the TLBO algorithm. The result of the flow curve is in-line with the response predicted in figure 18 and therefore it is not presented here. The assumed value of volume fraction of martensite and connectivity of the martensite is same for generating the artificial microstructure in both the cases of Voronoi-diagram, therefore, the proposed formulation is able to generate the artificial microstructure which is independent of the random number sequence used for the TLBO algorithm.

Figure 22. Effect of different class-size of TLBO on the microstructure.

Figure 23. Effect of different elite-size of TLBO on the microstructure.

5.7 Effect of input parameters of TLBO

The proposed algorithm for generating artificial microstructure of the dual phase steel is again checked for finding the sensitivity of input parameters of TLBO to the prediction of microstructure. The study is performed to find the effect of class-size and elite size. The volume fraction of martensite remains 10% and the connectivity of the martensite is kept at 0.20. The Voronoi diagram is generated using 1000 seed points, given in figure 3. The study is performed with class-size of 200 and 300. All other parameters are kept the same as detailed earlier. The resulting microstructure is presented in figure 22. It is observed that the sparsity of the martensite grains is different in both the microstructure. Subsequently, the model is applied for finding the effect of elite size on the predicted microstructure. All the parameters are kept the same except that the elite size used are 3 and 5. The resulting microstructure is presented in figure 23 and it is observed that the resulting microstructure is almost the same.

The generated microstructure with different class-size and different elite size are applied for the prediction of flow

stress of DP590 steel. The detailed procedure for the finite element analysis is already discussed in the previous sections. It is found that there is a negligible effect on the predicted flow curve due to the difference in class-size and difference in elite size for the TLBO algorithm. The results of the flow curve are in-line with the response predicted in figure 18 and therefore these are not presented here. It can be stated that the proposed formulation is able to generate the artificial microstructure which is independent of the input parameters used for the TLBO algorithm for the prediction of the flow curve of DP590 steel.

6. Conclusions

The micromechanical analysis of the dual phase steel using microstructure based RVE is the effective methodology for the estimation of its macroscopic properties. The microstructure generated using artificial methods is efficiently applied in a number of studies. The present work has proposed a new model for the generation of the

artificial microstructure of dual phase steel. The proposed model uses the Teacher-Learner based optimization (TLBO) technique with microstructure based controlling parameters viz. volume fraction and connectivity of martensite to predict the artificial microstructure. The generated artificial microstructure of the DP590 steel is applied to check the validity and applicability of the model for the estimation of macroscopic response under tensile loading. The model is able to predict the tensile stress–strain response with reasonable accuracy and there is a good agreement between the predicted and experimental response for DP590 steel. The model is able to capture the changes in the control parameters to the subsequent change in the artificial microstructure of the DP590 steel.

The study on the artificial microstructure obtained from the proposed model reveals that the increase in volume fraction with the same value of connectivity increases the dispersion of the martensite at some places whereas at other places the long-connected martensite is observed in the ferrite matrix. The increase in the connectivity of the martensite with the same value of volume fraction changes the shape and size of the martensite phase in the ferrite matrix. The significant change in the tensile macroscopic response is observed with the increase in the volume fraction in comparison to the connectivity of the martensite.

The novelty of the proposed model is that it is independent of the control parameters which are used to define the Voronoi-tessellation and the input parameters for the optimization algorithm. The model is only dependent on the material parameters which are used to define the microstructure of the dual phase steel. The model can be effectively and efficiently applied for the micromechanical analysis of dual phase steels. The model can be extended for getting the banded microstructure by the introduction of shape parameter [26] and further the model can be used to generate 3-dimensional (3D) artificial microstructure using 3D Voronoi-diagram.

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