Investigating the Effect of Cementite Particle Size and Distribution on Local Stress and Strain Evolution in Spheroidized Medium Carbon Steels using Crystal Plasticity-Based Numerical Simulations

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1. Introduction

Steel is widely considered as the most important alloy of iron and carbon due to its easy availability, high formability, low cost, and various applications.[1,2] In the automobile industry, steel is being used as an important raw material for varying strength and ductility needs.[3,4] On average, about 1.6 billion tons of steel are being produced annually.[5] Ferritic–pearlitic steel consists of alternate cementite and ferrite layers, which upon cold forming exhibit less uniform elongation due to present interstitial hard and brittle cementite. The spheroidization process driven by surface free energy is used to transform lamellar iron carbide (Fe₃C) into spheroidal morphology, which results in a material with remarkable combination of ductility and strength.[6–8] Typically, spheroidization is carried out in the automobile industry for steel sheets and bars subjected to cold working, i.e., rolling or forming.[9]

The global mechanical properties of a material depend upon the mechanical behavior of grains of phases present in it.[10,11] After spheroidization of C45EC steel with 0.45% carbon, the cementite grain size is usually small, i.e., in the range of 0.4–2.5 μm. Despite its small size, its shape and distribution in the ferrite matrix substantially...
affect the material’s strength and formability, as has been reported by the researchers in the past.[12–15] Various models have been proposed to study the influence of cementite morphology on the global mechanical properties of the low alloyed medium carbon steels.[13–15] Due to the pinning effect of fine cementite particles present in the middle of the ferrite matrix, the ferrite grains do not grow during spheroidization annealing (Zener drag effect).[14] Enhanced formability of spheroidized steels is attributed to larger ferrite grain size, reduced strain hardening exponent, and larger mean inter-particle spacing between the cementite particles.[16]

It was observed during micro-digital image correlations (µDIC) of multi-phase steel materials that plastic deformation takes place in the larger ferrite grains first and then proceeds toward smaller ones. Extreme localization of the strains is spotted at the boundary of heterogeneous grains.[17] It was suggested that better ductility could be achieved with hard second phase grains dispersion more homogeneously within the matrix.[18,19] The plastic deformation of the face-centered cubic (fcc) crystals by shear banding has been attributed to initial grain orientation and average grain size.[17] The strain path in the polycrystalline aggregate follows soft crystals, whereas the strain localization occurs at triple points or mostly on the grain boundaries (GBs).[20] A detailed analysis of a simplified model for a synthetic dual-phase microstructure was carried out by Woo et al.,[21] taking circular martensite with one orientation and ferrite with two orientations. He showed that the strain localization is strongly dependent on the grain orientations of the ferrite phase.

The microstructural importance of constituents in steel provides enough motivation to understand the effect of size, shape, and distribution of cementite on localized stress and strain behavior during deformation in medium carbon steels. There is a need to determine the exact response of the constituent particles in terms of their size and location for a specific material to get the desired mechanical properties by optimal resource utilization. This is important, because prolonged spheroidization may result in reduced strength of the material,[22,23] and is a time and energy-consuming process.[2,24,25]

2. Micromechanical Modeling

The simulation tool must be capable of predicting close to actual mechanical response of the material depending upon its constituent’s volumetric fraction, crystallographic texture, microstructure,[25] and process history used to synthesize it.[26,27] Various models that have been proposed from time to time for a better understanding of the crystalline materials are briefed in Table 1. The material models’ capability to predict the material response during deformation using simulation has progressed gradually to update the design process for real-time material application in the industry.

The major concern of computational science used for micromechanical simulation of crystalline materials is the cost of modern electronic equipment used in fast processing and time consumption required for solving coupled field equations at each material point. Based on the fundamental framework of the spectral method proposed by Moulinec and Suquet,[28] fast Fourier transform (FFT)-dependent solvers have provided time and memory-efficient tools for such simulations.[29] Advancements in mathematically robust models, such as an extension of the finite-element method (FEM) known as a spectral method, have been applied to many applications.[30–34] The simulation tool named DAMASK uses the same computational method for its modular hierarchy, which means it can quickly adapt multiple constitutive models along with the homogenization types, which is one of its main advantages.[35,36] It uses finite-strain theory coupled with the continuum mechanical description of deformable bodies to calculate the material response.[35,37] This tool has been used successfully to solve many problems, as detailed in the previous studies.[19,31,38–45] The recent steel matrix analysis with

| Model name                     | Merits/assumptions                                                                 | Demerits                                                                 | Ref.                      |
|--------------------------------|----------------------------------------------------------------------------------|--------------------------------------------------------------------------|---------------------------|
| Full constraint model          | Velocity gradient on the macroscale is the same on every grain at the microscale. | Lacks suitable prediction of strain at individual grain.                  | [56–59]                   |
| Relaxed constraint model       | It improves the satisfaction of stress equilibrium at GBs.                       | It cannot address the deformation processes other than plane strain deformation. | [57,60–62]               |
| Viscoplastic self-consistent   | The interaction between grain and a supposed medium around it has average constitutive behavior of the entire polycrystalline aggregate. | It just solves the non-symmetric tensors based on a complex mathematical model but does not produce better results. | [57,62]                   |
| model (VPCS)                  |                                                                                   |                                                                           |                           |
| Transformation kinetics model  | Includes the stress-state dependency of the phase transformation without requiring any restrictions on the magnitude of the stress invariants. | Involves 30+ parameters that are quite challenging to identify and need data training every time a different material batch comes. | [63–65]                   |
| LAMEL                         | It calculates the localized linkage between very adjacent grains by intense assessment of the stress equilibrium at the GBs. | Designed only for rolling process and for material with flat elongated grains. | [29,57]                   |
| Dislocation-based strain       | One parameter within the model is associated with the dislocation mean free path and related in each case to a characteristic microstructural feature. | It is a homogenized model and only yields averaged stress–strain response of the material. | [66,67]                   |
| hardening model               |                                                                                   |                                                                           |                           |
| Crystal plasticity finite-element model (CPFEM) | Considers both stress equilibrium and strain compatibility so better than almost all the previous homogenization schemes. | Computationally extremely costly. Needs the most time and other advanced material resources. | [29]                      |

Table 1. Comparison of various models for understanding and simulation of micromechanical behavior of grains in polycrystalline materials.
ceramic particles by Qayyum et al.\cite{46} has shown the viability of the DAMASK code to conduct a local deformation behavioral analysis.

This research aims to investigate plastic behavior in spheroidized medium carbon steels by numerical simulation using DAMASK. In particular, the influence of the cementite particles size, location, and percentage distribution in the ferrite matrix is investigated. The overall mechanical response of the material upon application of the tensile load is studied based on local stress and strain distribution maps.

3. Experimental Setup and Microstructure Characterization

The experimental setup for investigating the mechanical behavior of medium carbon steel under consideration (C45EC) has been carried out separately and published elsewhere\cite{13}. The chemical composition of this steel is shown in Table 2. The volume fraction of cementite for 0.45 wt% carbon is $\approx$7%.

A coarse lamellar ferritic-pearlitic microstructure was obtained before spheroidization by austenitizing 10 mm diameter and 100 mm long steel rods at 900 °C for a quarter of an hour followed by air cooling to room temperature. Spheroidization of samples was carried out using an inter-critical annealing at 740 °C for 1 h, followed by soaking at 680 °C for 12 h. After etching with a 3% Nital solution, the samples were examined under the scanning electron microscope (SEM) for recording microscopy images at different magnifications.

For tensile testing, 20 mm gauge length cylindrical samples were manufactured according to the standard DIN EN 6892-1. These spheroidized samples were subjected to a tensile loading at 0.05 mm s$^{-1}$ crosshead speed. The tests were carried out using an AG100 uniaxial material testing machine. The recorded high-resolution force–displacement data were processed to plot experimental true stress–strain curves used for the calibration of simulation model.

A series of microscopy images at various magnifications have been shown to explain the geometrical attributes more clearly for both phase grains concerning their respective sizes present in the material. In Figure 1a, the cementite particles seem to exist in the banded format. On further magnification of these zones, it is observed that they are heterogeneously distributed within these bands. The SEM images show the cementite particles with varying sizes clustered at various places in Figure 1b,c. Ferrite grains are labeled “F” in this figure.

The cementite particles being relatively small are shown in the more magnified image, where their two distributions mutually dissimilar in size can be observed. A different bimodal distribution is found at this magnification for cementite particles located at the GBs and inside the ferrite grains. The comparatively large cementite particles are seen clustered at specific places represented by “C$_S$” (Figure 1c). Simultaneously, various cementite particles with large aspect ratios can be seen with little contrast in geometrical shapes. The other area of interest, along with these clinkers, is the presence of small-sized cementite particles referred to as “C$_L$” in Figure 1c. The overlapping at some positions is observed due to 2D visualization of the 3D cementite particle distribution. A few clinkers of cementite are also present, having an aspect ratio up to 1:8, which seems to be a product of incomplete spheroidization, and hence not considered for simulation data input. The geometrical attributes of the ferrite and cementite phases are quantified by processing Figure 1c, using the ImageJ software\cite{47}.

After carefully measuring the cementite particles (14 grains from C$_L$ cluster and 32 grains from the C$_S$ cluster), the generated statistical data are shown in Table 3. This size distribution data were used for the generation of virtual representative volume elements (RVEs) in Dream.3D.

![Figure 1. Microscopy images of 83% spheroidized C45EC at different magnifications.](image)

Table 2. Chemical composition of the investigated steel in weight percentage.

| Elements | C | Si | Mn | P | S | Cr | Mo | Ni | Al | Cu |
|----------|---|----|----|---|---|----|----|----|----|----|
| Wt%      | 0.44 | 0.10 | 0.75 | 0.007 | 0.017 | 0.04 | 0.011 | 0.04 | 0.03 | 0.03 |

Table 3. The statistical data calculated using image analysis software (ImageJ) from the microscopy image.

| Particle type | Average equivalent diameter [μm] | Minima [μm] | Maxima [μm] | Standard deviation for diameter [μm] |
|---------------|----------------------------------|-------------|-------------|-------------------------------------|
| C$_S$         | 0.804                            | 0.398       | 1.633       | 0.302                               |
| C$_L$         | 1.582                            | 1.028       | 2.598       | 0.436                               |
| F (matrix)    | 13.78                            | 8.704       | 22.265      | 3.563                               |
3.1. Numerical Simulation Modeling

The numerical simulation task demands some robust and modern tool, which can consider the grain level mechanics of the material and relate it to the component level design parameters based on the input microstructural details. The method of experimental determination of microstructural details of the polycrystalline material has its own associated challenges. An electron backscatter diffraction (EBSD) analysis performed on an SEM is a well-known process to capture the effect of the thermomechanical processing route on crystallographic texture. However, a 2D virtual microstructure using an RVE generation tool is used in this study. These RVEs are easier to construct, offer a wide range of parametric studies, and can be used to compare the results with localized deformation behavior at various sections. The virtually generated inverse pole figure (IPF) maps of virtually generated RVEs are shown in Figure 2.

The typical approach of RVE simulations for investigating a material during deformation is to observe the localized mechanical response of an RVE subjected to the well-defined boundary conditions, which is then extrapolated to the whole material. This demands the RVE to be necessarily a representative of the whole material and behave likewise when virtually loaded. The micromechanical response of any material is defined using phase parameters for individual phases determined using advanced techniques. Ferrite and cementite phase parameters have been previously reported and used to evaluate the micro-level stress and strain partitioning during such simulations.

For the complete description of a polycrystalline material for crystal plasticity (CP) simulation, generally, the phase parameters for both elastic and plastic deformation of all the phases present in it are specified. Due to a considerable mismatch in the plastic behavior of ferrite and cementite, the latter is assigned only elastic properties here. The fitting parameters can be different for the same grade steels because of the dissimilarity in manufacturing routes and other factors. Therefore, fitting parameters are calibrated by comparing simulation results with experimental observations. The modified ferrite phase parameters used in this study, along with elastic phase parameters of cementite, are presented in Table 4.

In the numerical simulation model, all RVEs are subjected to the quasi-static uniaxial tensile loading at a strain rate of $10^{-3}$ s$^{-1}$ up to an overall global strain of 20%, in principle, x-direction. The phenomenological model for the current simulations is adopted from the work of Roters et al. The total deformation gradient comprises of elastic and plastic parts

$$F = F_e F_p$$

where $F_e$ is the elastic rotation and stretching, whereas $F_p$ is the deformation gradient due to the dislocation slip. The elastic tensor in the model is calculated as

$$E_e = \frac{1}{2} (F_e^T F_e - I)$$

Figure 2. IPF maps for all the nine synthetic microstructures, elaborated by their case code (left) and percentage concentration of cementite particles on the ferrite grain boundaries (top). The white spherical dots in all the RVEs are representing the places of cementite grains. The orientations of the cementite particles cannot be viewed profoundly because of their small size, therefore, ignored here.
The hardening rule implemented in this study is as follows:

\[ S = C E_e = F_c^{-1} \left( \det F_c \right) \sigma F_c^{-T} \]

where \( C \) is the elastic stiffness tensor, and \( \sigma \) is the Cauchy stress tensor. The evolution of the plastic deformation gradient is defined as

\[ \dot{F}_p = L_p F_p \]

Plastic velocity gradient \( L_p \) is caused by dislocation slip and is stated as

\[ L_p = \dot{\gamma}^\alpha (m^\alpha \otimes n^\alpha) \]

where \( \dot{\gamma}^\alpha \) is the shear rate on the slip system \( \alpha \) with slip directions \( m^\alpha \) and slip plane normal \( n^\alpha \). The crystallographic orientation of the individual grain is responsible for activating slip systems upon application of load. This slip-plane and slip-direction activation energy is supplied by the inherent behavior associated with individual crystal structures depending upon their axes parameters.

The shear rate due to dislocations over the slip systems \( \alpha = 1, \ldots, N_{\text{slip}} \) is defined as

\[ \dot{\gamma}^\alpha = \dot{\gamma}_0 \left( \frac{\tilde{\gamma}^\alpha}{S^\alpha} \right) \text{sgn}(\tilde{\gamma}^\alpha) \]

The reference shear rate \( \dot{\gamma}_0 \), the exponent \( n \) is stated in Table 4. The hardening rule implemented in this study is as

\[ S^\alpha = h_0 \left( 1 - \frac{S^\alpha}{S^\alpha_0} \right)^w q_{\text{diff}} |\dot{\gamma}^\alpha| \]

where \( h_0 \) is the reference hardening parameter, and \( S^\alpha_0 \) is the saturation stress that is constant for each slip system family. The values for the model parameters were adopted from already published data, and some fitting parameters were calibrated to match the material flow curve obtained experimentally following an already reported methodology.[51] For further details of the CP formulation used to evaluate the localized mechanical response of elastic–viscoplastic material, readers are encouraged to read the work of Tasan et al.[38]

### 3.2. Isotropic Simulations

A methodology developed to identify the isotropic material behavior was adopted from already published work.[51] The scheme takes a 3D RVE with 10 × 10 × 10 dimensions having grains with random crystallographic orientations in all directions. This small volume element is first ensured to behave in an isotropic manner by applying load in three orthogonal directions. In comparison with the stress–strain curve of 83% spheroidized C45EC samples, the results of these simulations are shown in Figure 3. The calibration of the material model with anisotropic volume element after matching of trend yields improved values for fitting parameters of the ferrite matrix. The updated model with calibrated

![Figure 3](image_url)

**Figure 3.** True stress–strain plastic flow curve of medium carbon steel. Comparison of tuned material model behavior with experimental observation after loading in three principal directions.

| Parameter definition | Parameter symbol | Value [ferrite] | Modified value [ferrite] | Value [cementite] | Unit |
|----------------------|-----------------|----------------|--------------------------|-----------------|------|
| First elastic stiffness constant with normal strain | \( C_{11} \) | 233.3 | – | 375.0 | GPa |
| Second elastic stiffness constant with normal strain | \( C_{12} \) | 135.5 | 235.5 | 161.0 | GPa |
| First elastic stiffness constant with shear strain | \( C_{44} \) | 128.0 | – | 130.0 | GPa |
| Shear strain rate | \( \dot{\gamma}_0 \) | 1 \times 10^{-3} | 5.6 \times 10^{-4} | – | m s^{-1} |
| Initial shear resistance on [111] | \( S_0 \) [111] | 95 | – | – | MPa |
| Saturation shear resistance on [111] | \( S_\infty \) [111] | 222 | – | – | MPa |
| Initial shear resistance on [112] | \( S_0 \) [112] | 96 | – | – | MPa |
| Saturation shear resistance on [112] | \( S_\infty \) [112] | 412 | – | – | MPa |
| Slip hardening parameter | \( h_\text{slip} \) | 1 | – | – | – |
| Interaction hardening parameter | \( h_\text{int} \) | 1.0 | – | – | – |
| Stress exponent | \( n \) | 20 | 3 | – | – |
| Curve fitting parameter | \( W \) | 2.25 | 2.0 | – | – |
parameters was implemented in the DAMASK framework for full phase numerical simulation of the RVEs.

### 3.3. Full Phase Simulations

The Dream.3D\textsuperscript{[52]} software package is used to construct the virtual microstructure by adjusting the grain size statistics separately for both phases. This software uses its default “statistics generator filter” to take input data sources and creates the probability distribution of the data. In particular, maxima, minima, standard deviation, and mean diameters of the particles are used at input data. These values were carefully determined using the ImageJ software to ensure that the virtually made microstructures do not differ much from the actually observed microscopy images. The RVEs slightly vary due to constraints of packing the secondary phase particle within the matrix during synthetic microstructure generation.

The dimensions of all RVEs for full phase simulations are set $400 \times 400 \times 1 \, \mu m^3$, divided into $400 \times 400 \times 1$ mesh points. The suitable optimum dimensions are needed to be selected for simulation; i.e., it should be large enough to behave in a manner the whole material would behave. Simultaneously, the dimensions must be small enough, which can be simulated utilizing optimum computational time and processing equipment. The software generates an output file defining the geometrical attributes of grains in the generated RVE with information of microstructural texture and geometrical aspects for individual grains. Additional information on homogenization, crystallite, and phase properties is incorporated in the material configurations file to make it readable for DAMASK. The tensile load in the $x$-direction with a strain rate of $1 \times 10^{-3} \, s^{-1}$, mixed boundary conditions, and a $3 \times 3$ deformation gradient tensor $\mathbf{F}_{ij}$ is defined as stated in Equation (8).

$$
\mathbf{F}_{ij} = \begin{bmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{bmatrix} \times 10^{-3} \, s^{-1} \tag{8}
$$

The $3 \times 3$ first Piola–Kirchhoff stress tensor $\mathbf{P}_{ij}$ needed as an output in the tensile load response applied to each material point is also defined as Equation (9).

$$
\mathbf{P}_{ij} = \begin{bmatrix}
* & * & * \\
* & 0 & * \\
* & * & 0
\end{bmatrix} \, Pa \tag{9}
$$

The coefficients of both the tensors shown with “*” are the complementary conditions imposed on the material for input and output. To study the effect of varying morphology of cementite particles on the overall material response, the scheme of the study has been devised with much care to cover maximum aspects. The size and distribution of the second phase particles observed in Figure 1 are the physical variables expected to have majorly contributed to the global mechanical response.

Therefore, two aspects, namely, size and distribution of cementite particles, are intended to be analyzed for this problem.

1) Three size schemes are selected to generate the microstructures virtually for CP simulation. First, only small-sized cementite particles ($C_3$), second, the cementite particles with a somewhat large size ($C_4$), and third, the consideration of both small-sized and large-sized cementite particles together which is named as bimodal ($C_5$ and $C_3$) (see Figure 1); 2) Each of these three schemes has been further simulated three times individually for different percentage locations of the second phase particles on the ferrite grain boundaries, i.e., 0%, 50%, and 95%.

In this way, the nine cases simulation set for the analysis of the influence of the cementite particles with the variation of size and distribution within the ferrite matrix has been executed, as detailed in Table 5. The crystallographic orientations for all the cases for individual grains of ferrite phase generated in the software are given by IPF maps (see Figure 2).

### 4. Results

The results of the simulation in comparison with the experimental stress–strain curve are shown in Figure 3. The flow curve is separated into two zones, A and B. It is evident that the RVE, when loaded in three different directions, behaves isotopically, and matches well with the experimental data. In zone A: the simulation model overpredicts the total stress in the material. This overestimation possibly occurs due to the absence of the grain boundary consideration in the numerical simulation model. Complex dislocation movement initiated by the various active slip systems, dislocation pinning, and locking takes place in the material during the actual application of tensile load. This continues until the onset of yield at the end of zone A, whereas the simulation results do not show this behavior due to the absence of these definitions in the model. In zone B: from 5% to 20% of true strain, the simulation results of the calibrated model match well with the experimental observations ($<3\%$ error). The model is expected to predict the plastic behavior of the material in this zone perfectly. After this zone, the material strength increases due to local strain hardening, eventually, the load-bearing capacity of the material degrades and failure occurs.

| Case code | Cementite particle/grain configuration | Equivalent sphere diameter [μm] | Maxima/ minima/ sigma [μm] | Concentration of cementite on ferrite GB [%] |
|-----------|---------------------------------------|-------------------------------|---------------------------|------------------------------------------|
| Sm – 0 | Small | 3.1 | 6.3/1.1/0.2 | 0 |
| Sm – 50 | Sm – 95 | | 0 | 50 |
| La – 0 | | Large | 4.9 | 8.1/2.9/0.2 | 0 |
| La – 50 | | | 0 | 50 |
| La – 95 | | | 0 | 95 |
| Bi – 0 | | | 0 | 50 |
| Bi – 50 | | Bimodal | 4.0 | 8.1/1.1/0.2 | 0 |
| Bi – 95 | | | 0 | 95 |
| Fe | Ferrite (matrix) | 19.6 | 31.1/10.8/0.2 | – |
4.1. Local Stress and Strain Maps

Local stress distribution in all constructed RVEs at 20% true plastic strain is shown in Figure 4. In all cases, the stress carried by the cementite particles is much higher (≈13 GPa) as compared with the stress in the ferrite matrix (≈500 MPa). Due to very high-stress values, the cementite particles are not represented in the figure as they distort the scale.

Stress is higher in grains that are not aligned in the plastically favorable orientations to the deformation direction. Visually, the stress is lowest in small cementite particles and highest in the case of large cementite particles. The stress distribution becomes more homogenized, with the particle distribution moving toward the grain boundaries. It can also be observed that the stress concentration is higher in zones with more concentration of cementite particles. The stress distribution is generally observed as a significant contrast in the whole map, where some grains hold considerable stress. In contrast, some possess very low stress, as represented with the blue color in Figure 4.

At 20% of the true plastic strain, the local strain maps of all RVEs are given in Figure 5. Although the strain distribution is heterogeneous, the highest amount of strain is observed in the small cementite particle RVEs. Lower strain in the matrix is observed in large cementite particle RVEs. Figure 4 and 5 show that the highest stresses are present in the cementite particles with the highest strain existing on the ferrite/cementite interface. It is also observed that the morphology and distribution of the cementite particles widely affect the local stress and strain distribution in the material during deformation. Although evident from observing the maps physically, yet this effect is impossible to compare with local stress and strain maps of all the cases accurately, due to several probable reasons described in Section 4.

4.2. Stress and Strain Evolution

It is observed that no substantial difference exists in all cases concerning stresses, but marginal differences are observed with Bi-0 case showing the highest local stress values and the Sm-50 case at the lowest end. Along with presenting the local stress and strain maps of all the cases where a general comparison can be seen, it is also interesting to have an in-depth insight into the evolution conditions for the cases of simulation with extreme (lowest and highest) stress distribution shown in Figure 6 and 7.

The stress distribution at 5% global strain seems to have initiated with the wider patches shown with green colors in Bi-0 case, whereas in Sm-50, these patches are relatively suppressed. The evolution of the stresses in all the RVEs is observed to propagate diagonally in the ferrite grains (from upper-left to the bottom-right corner). The same fashion continues initiating from 5% strain and dominates up to 20% of the global strain.

In each strain distribution map, it is evident that higher strains initiate at the interface of the ferrite and cementite phases and continue to grow. Differently sized cementite

![Figure 4. Stress distribution maps of the RVE at 20% of true plastic strain applied in the horizontal direction on all RVEs.](image-url)
particles have different responses, small particles in Sm-50 at 20% strain assist in broad distribution strains, and no dark red colored regions are seen as in Bi-0 at 20% strain. Similarly, for the local strain distribution, these extreme cases have their specific characteristics. The less concentrated stressed points in Bi-0 case have undergone more localized strains at 20%
global strain. Likewise, the points that have fewer stresses at the final map for Sm-50 in Figure 6 can be seen to have undergone more strains in Figure 7.

4.3. Local Stress and Strain Probability Distributions

Evaluating the microstructural data to determine the structure–property relationship using DAMASK offers the opportunity to familiarize with the fundamental underlying mechanisms taking place for plastic deformation in the RVE. Simultaneously, it poses a significant challenge to represent the data in a more presentable and statistically unambiguous and unequivocal way. The data presented with the help of probability density function (PDF) and cumulative distribution function (CDF) provide relative quantitative insight into the material properties at about 20% strain. The ferrite phase histograms are shown in Figure 8a,b. These figures represent true strain in percentage and true stress in Pascal.

Figure 8 shows that the maximum stress points are located around 0.6 GPa within a range of 0.3–0.9 GPa for both Sm-0 and Sm-95. For Sm-50, the maximum stress points are at about

Figure 7. Maps for the evolution of local strain distribution for extreme (lowest and highest) of the nine cases showing stress evolution during deformation for 5%, 10%, and 20% of the global strain values.

Figure 8. PDF and CDF for the small cementite particles plotted against the true strain at 20% global strain.
0.5 GPa, whereas the distribution is relatively wider. It is observed that the stress and strain distribution are heterogeneous. The small cementite particle cases, 0%, 50%, and 95% concentration on the ferrite grain boundaries, show a peculiar behavior. In Sm-50 case, cementite particles with comparatively low values of stress and strain are observed while the cases Sm-0 and Sm-95 show an increasing trend both in stress and strain.

The histograms shown in Figure 9a,b, display the cases for La-0, La-50, and La-95. The maximum stress points are located around 0.6 GPa for the ferrite phase again, but the La-50 shows a more heterogeneous response. La-50 is located at the low stress and low strain regions, whereas La-0 and La-50 show the trend same as for small cementite particles. Increasing trend of true strain and true stress from La-0 to La-95 is observed.

Figure 9. PDF and CDF for the large cementite particles plotted against the true strain at 20% global strain.

Figure 10. PDF and CDF for the bimodal cementite particles plotted against the true strain at 20% global strain.
The ferrite phase response for the bimodal distribution of cementite particles is shown in Figure 10a,b. The histograms show different behavior than the small and large cementite particle individual cases. The strain distribution trends for Bi-0, Bi-50, and Bi-95 are in the decreasing order for ferrite grains. The maximum stress points are located around 0.6 GPa for the ferrite phase again, but the Bi-0 shows a more stressed configuration response. Bi-95 is located at the low stress and low strain regions, whereas Bi-0 and Bi-50 show the increasing trend.

5. Discussion

In this research, the CP-based numerical simulation model in the framework of DAMASK was adopted to simulate global and local deformation behavior of spheroidized steels. The material model was calibrated by adopting an already developed, benchmark-based RVE approach. The phenomenological-based material model was adopted from the previous studies.[18,51] Slip rate and fitting parameters $n$ and $w$ were modified and assumed calibrated when found matching up to 97% by comparing it with experimental tensile test results of the same material. Due to the very high stiffness of cementite particles, they were assigned only elastic properties. The comparison of global stress and strain curve with less resolved 3D material RVE is shown in Figure 3. There is a good match of the plastic deformation from 5% to 20% of true plastic strain. At zone, “A” material undergoes complex grain boundary motion and interlocking phenomena, whereas the simulation model lacks this description. To further improve results, there is a need to introduce some modifications, i.e., the orientation distributions function (ODF) might play a role. Therefore, ODF of the material measure by X-ray diffraction should be adopted for global results, which is a task of future research.

When the simulation results are compared with the previous work of similar nature,[19] the trends and observations look similar. The globally tuned model was then used to simulate local material behavior. The RVEs were developed using the statistically measured microstructural data from material microscopy images. The problem has been schematized in nine different cases considering 0%, 50%, and 95% concentration of cementite particles on matrix grain boundaries with three different size configurations of cementite particles. This has been done to understand the contribution of the cementite particle size and distribution on the mechanical properties of spheroidized steels. The simulation results of local stress and strain distribution after 20% of the true strain are shown in Figure 4 and 5. It is observed that due to the changing morphology and distribution of cementite particles, the areas of high stress and strain change significantly. These high-stress zones may result in brittle particle cracking and void formation, whereas the high strain zones assist in void consolidation, failure initiation, and propagation,[18,53] resulting in eventual failure of the material.

Strain distribution is observed more concentrated in areas where closely existing cementite particles are dominantly populated (see Figure 5). It is also observed that with increasing second-phase particle size, strain distribution becomes less localized; this has been reported by researchers in the past as well.[54] Qualitative results can be well compared with the previously reported results,[18] but, quantitatively, the results might be misleading due to some assumptions, i.e., 2D RVE consideration, spherical cementite particles shape, perfect grain boundary and phase interface.

![Figure 11. PDF and CDF for the small, large, and bimodal cementite particles plotted against the True Strain in percentage at 20% global strain.](image-url)
RVE geometry, perfect interface, and no-slip of grain boundary and 13 GPa and between 0.03 and 0.045, respectively. Cementite particles are all over the place and range between 9 distributions better. It is observed that stress and strain in Figure 11 to visualize and compare the local stress and strain and CDFs have been plotted on top of each other in distributions visually for the same total stress or strain is the ferri-stress strain distribution in RVEs. It is observed that there is a significant difference in the stress and strain distributions. The other strain distribution for individual phases to quantitatively compare local stress and phases in heterogeneous formation is analyzed using a CP-based DAMASK, presents a cost-effective and fast possible solution for such analysis; 3) The full phase simulations are only qualitatively accurate due to the 2D RVE consideration compared with the 3D physical nature of the material; 4) When orientation distribution is not the same in RVEs, the analysis of microstructural deformation data using PDFs and CDFs is a helpful method for quantitative comparison and extraction of useful trends from full phase simulations with comparable grain size.

Statistical comparison was made using probability and CDFs for individual phases to quantitatively compare local stress and strain distribution in RVEs. It is observed that there is a significant difference in the stress and strain distributions. The other factor affecting the direct comparison of local maps and statistical distributions visually for the same total stress or strain is the ferrite grains orientation dissimilarity in each RVE. All the PDFs and CDFs have been plotted on top of each other in Figure 11 to visualize and compare the local stress and strain distributions better. It is observed that stress and strain in cementite particles are all over the place and range between 9 and 13 GPa and between 0.03 and 0.045, respectively.

The stresses in ferrite and cementite are relatively high. They seem non-realistic, which is due to the considered 2D RVE geometry, perfect interface, and no-slip of grain boundary assumptions, resulting in the overestimation of the values. In the current cases of changing cementite morphology and distributions, it is difficult to plot trends of the effect on the overall material behavior. This is because if these are plotted (refer to Figure 12), a large scatter in the data is observed.

6. Conclusion

In this research, the local deformation behavior of 83% spheroidized medium carbon steel having ferrite and cementite phases in heterogeneous formation is analyzed using a CP-based numerical simulation model. RVEs with varying cementite particle sizes and distributions were constructed using DREAM.3D. The statistical data for the construction of RVEs were measured from microscopy images of well-prepared samples. The study has provided a detailed insight into the factors affecting the maximum local strain distribution in multi-phase spheroidized steels, which can help choose optimal spheroidization degrees in the future. The study can be concluded as follows.

1) The identified parameters can satisfactorily predict the flow stress in the 83% spheroidized C45EC steel with an accuracy of ≥97% in a 5–20% true strain range; 2) The proposed methodology in the article for analyzing microstructural data from microscopy images, using that data to construct virtual microstructures of spheroidized steel and running full phase simulations using DAMASK, presents a cost-effective and fast possible solution for such analysis; 3) The full phase simulations are only qualitatively accurate due to the 2D RVE consideration compared with the 3D physical nature of the material; 4) When orientation distribution is not the same in RVEs, the analysis of microstructural deformation data using PDFs and CDFs is a helpful method for quantitative comparison and extraction of useful trends from full phase simulations with comparable grain size.

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Conflict of Interest

The authors declare no conflict of interest.

Keywords
crystal plasticity, local deformation behavior, numerical simulation, spheroidized steel, statistical distribution, stress and strain

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