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Published in:
Engineering Fracture Mechanics

DOI:
[10.1016/j.engfracmech.2019.106683](https://doi.org/10.1016/j.engfracmech.2019.106683)

Published: 01/11/2019

Document Version
Peer reviewed version

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Please cite the original version:
He, J., Piao, Z., Wang, X., Lian, J., & Münstermann, S. (2019). Micromechanical modeling of cleavage fracture for a ferritic-pearlitic steel. *Engineering Fracture Mechanics*, 221, [10668].
<https://doi.org/10.1016/j.engfracmech.2019.106683>

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PII: S0013-7944(19)30407-2

DOI: <https://doi.org/10.1016/j.engfracmech.2019.106683>

Reference: EFM 106683

To appear in: *Engineering Fracture Mechanics*

Received Date: 30 March 2019

Revised Date: 19 September 2019

Accepted Date: 19 September 2019

Please cite this article as: He, J., Piao, Z., Wang, X., Lian, J., Münstermann, S., Micromechanical modeling of cleavage fracture for a ferritic-pearlitic steel, *Engineering Fracture Mechanics* (2019), doi: <https://doi.org/10.1016/j.engfracmech.2019.106683>

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Micromechanical modeling of cleavage fracture for a ferritic-pearlitic steel

Jinshan He^{1,2}, Zhengyin Piao², Xitao Wang^{1*}, Junhe Lian^{2,3*}, Sebastian

Münstermann²

1. Collaborative Innovation Center of Steel Technology, University of Science and Technology Beijing, Beijing 100083, PR China

2. Steel Institute, RWTH Aachen University, 52072 Aachen, Germany

3. Department of Mechanical Engineering, Aalto University, Puumiehenkuja 3, 02150 Espoo, Finland

Abstract

Despite efficient computational capability of phenomenological macromechanical models to predict cleavage fracture, they still lack microstructure sensitive information for material design. Therefore, a microstructure-based micromechanical modeling approach is proposed to predict cleavage fracture for a steel of grade AISI 1045 at different stress states. For the micromechanical modeling, virtual experiments are performed on an artificial microstructure model to derive the plasticity and cleavage damage initiation strain for the investigated material at -196°C. The predicted microcrack initiation strains of cleavage fracture at two different states (plane strain tension and equibiaxial tension) agree well with the calibrated results of macromechanical modeling, illustrating the validity and predictive capability of the proposed approach. Furthermore, the approach is applied to a microstructure sensitivity study on artificial microstructure models with different microstructure constituents to investigate the influence of microstructure on the behavior of cleavage fracture.

Therefore, the new approach is contributing to the material design directly.

Keywords: cleavage fracture, micromechanical modeling, artificial microstructure model, stress state, scale bridging.

* Corresponding authors.

Xitao Wang

Tel.: +86-010-62332789; Fax: +86-010-62336898;

E-mail address: xtwang@ustb.edu.cn

Junhe Lian

Tel.: +358 50 477 0765

E-mail address: junhe.lian@aalto.fi

1. Introduction

With the rising applications of structural steels at low temperature, cleavage fracture, which happens without any warning signal, draws increasing attention [1, 2]. For safety assessment, several phenomenological macromechanical models have been developed to predict component failure [3-6]. For instance, the Beremin group proposed a model with integrated principal stress in the plastic volume to describe the probability of cleavage fracture [3]. The model has been successfully used to predict the fracture toughness on the lower shelf of a reactor pressure vessel steel of grade A508 [7]. With enhanced cleanliness of modern steels, a considerable number of models have considered the plastic strain to initiate microcrack as another significant parameter for the prediction of cleavage fracture. Kroon et al. have applied an exponential function of plastic strain and a non-local stress measure to describe the probability of nucleation and propagation of microcracks, respectively [4]. More recent studies have further taken the effect of stress triaxiality into account for cleavage fracture prediction [5, 6]. Recently, inspired by the development in the ductile fracture models [8, 9], a generalized Orowan model has been introduced to consider the influence of plastic strain and stress state on the cleavage fracture behavior [10]. The model introduces the stress-state-dependent microcrack initiation strain to further develop the classical Orowan criterion, due to the observation of unexpected, but pronounced plasticity at -196°C . The model achieved good predictive capability on cleavage fracture behavior in a large stress state range. Owing to their high efficiency of computation and easy implementation, those macromechanical models are widely applied to the simulation

of various mechanical tests. However, it is difficult to apply them to material design since they fail to link microstructure and damage behavior. Therefore, it is necessary to develop micromechanical models for cleavage fracture containing microstructure information, like phase fractions, grain size distributions and so on.

Micromechanical modeling can be employed to study the effect of microstructural features on cleavage fracture by generating an artificial microstructure model. To conduct micromechanical modeling, representative volume elements (RVE), a sub-sized volume which can describe microstructural features of investigated materials, are usually applied. Generally, there are two approaches to generate RVE. One method refers to the direct mapping from the micrograph of material [11], allowing an immediate comparison between simulated and experimental results [12]. But the generated RVE can just present the local properties of material because the simulated results are mostly restricted to the mapped regions. Instead, another approach applies the statistical information of real microstructure to generate an artificial microstructure. Although it is difficult to find the generated microstructure in the real sample, the mean properties of material can be precisely presented with the model.

The micromechanical modeling approach has been applied to many studies correlating the microstructure features, specifically texture, with the plastic anisotropic properties [13-15]. Along with suitable damage criteria, micromechanical modeling with the generated RVE can be performed to analyze different types of failure for steels [16, 17]. Lian et al. initially employed the maximum force criteria on the constructed RVE to predict ductile damage initiation for a dual-phase (DP) steel [16]. The determined

damage initiation strain agreed well with the experimental results and it revealed that the initiation of damage on a micro level results from the heterogeneous nature of the microstructure. This approach was further successfully applied to a ferritic-pearlitic steel for the prediction of ductile damage initiation [18]. With regard to the micromechanical modeling of cleavage fracture, Mathieu et al. have generated realistic three-dimensional RVE based on morphological information of the A508 bainitic steel [19]. They set up a suitable calibration process for the identification of a crystal plasticity model of the steel. Although a fracture criterion at the grain level is applied to provide a new statistical description of cleavage fracture in the study, the results are not compared to experimental ones to illustrate the predictive capability of this approach. Moreover, the extension of the method to a wide range of stress states has not been achieved yet.

In the present work, a micromechanical model to predict the cleavage fracture at -196°C under two different states (plane strain tension and equibiaxial tension) for a steel AISI 1045 is presented. For the construction of the model, RVEs based on statistical microstructure information are generated by an in-house platform. Afterwards, the plasticity laws of ferrite and pearlite are calibrated by tensile tests at -196°C and assigned to the corresponding constituents in the RVEs. Finally, different boundary conditions are imposed on the RVEs and a local cleavage fracture criterion is applied in post-processing to extract the microcrack initiation strain. To validate the proposed approach, the extracted strains from the micromechanical simulations are compared with the calibrated results of the generalized Orowan model [10]. In addition, a

microstructure sensitivity study is also performed to investigate the influence of phase fraction on the behavior of cleavage fracture.

2. RVE generation

2D RVEs with small thickness were generated by using an in-house platform in this work. The details of generating the RVE has been introduced in reference [18]. To describe the plasticity of ferrite in this article, the crystal plasticity (CP) model is applied, of which the constitutive equations are on the basis of 3D stress tensor [20]. In this case, only the boundary condition of plain strain is applicable using 2D RVE, which is not acceptable in this work. Although the cubic 3D RVE is a potential solution to simulate more complex stress states, the seeding and tessellation methods for generation of 3D RVE are too complex to be realized. Also, the computational efficiency of simulation will decrease significantly due to huge quantity of elements. Therefore, the final scenario is designed as 2D RVE plus a small thickness, or called simplified 3D RVE. Compared with the cubic 3D RVE, only limited decrease of computational efficiency is caused by simplified 3D RVE, since the number of elements keeps constant as that of 2D RVE. Under the plane stress conditions, more stress states can be simulated using simplified 3D RVE than that of 2D RVE. Thus, the simplified 3D RVE is a feasible solution when taking the current conditions and methods into account. To generate RVEs, the microstructure information of the steel AISI 1045 was analyzed with an optical microscope, as shown in Fig. 1. The investigated material is a normalized medium carbon steel which is delivered as a round bar with 100 mm diameter. The microstructure was also investigated on different locations and directions

of the round bar, and the difference resulting from segregation is insignificant. According to the statistical analysis of a figure of 200:1 magnification, the steel is composed of 43 vol.-% ferrite (white region) and 57 vol.-% pearlite (dark region) respectively. Since the few inclusions do not play a significant role during the process of cleavage fracture, they are not taken into account for the construction of RVEs [21]. Statistical analysis of several hundreds of grains was conducted as seen in Fig. 2. Obviously, the histograms for both of the grain size distribution show positive skewness. Hence, the gamma distribution function is applied to describe the distribution:

$$f_{gamma}(x) = \frac{1}{\beta^\alpha \Gamma(\alpha)} x^{\alpha-1} e^{-\frac{x}{\beta}}, x > 0, \quad (1)$$

where α and β denote the shape and scale parameters respectively; $\Gamma(\alpha)$ is the gamma function of α [22]. The fitted parameters are shown in Table 1. To check for the significance of the statistical function, the Kolmogorov–Smirnov test has been performed here [23]. In general, this test evaluates the overall deviation $D_{\max}$ between data obtained by statistical analysis and the calibrated distribution function. A sufficient degree of significance is achieved for $D_{\max} = 0.032$ and 0.039 for ferrite and pearlite respectively since they are both smaller than their critical values.

Fig. 1. The microstructure of steel AISI 1045.

Fig. 2. Grain size histogram with gamma distribution function for (a) ferrite and (b) pearlite in steel AISI 1045.

Table 1. Summary of fitted parameters for gamma distribution functions.

Phase	α	β
Ferrite	5.52	2.31
Pearlite	3.58	4.20

Based on the microstructure information, the periodic artificial microstructure model with the size of $200\ \mu\text{m} \times 200\ \mu\text{m}$ was generated by multiplicatively weighted Voronoi tessellation, as shown in Fig. 3. Since there is no significant texture found in the steel by EBSD analysis [18], the orientations of different ferrite grains are assigned randomly. The interface between ferrite and pearlite is assumed to be perfect in the RVE. The $200\ \mu\text{m} \times 200\ \mu\text{m}$ area RVE contains approximately 130 grains in total, which is enough to represent the microstructure of the investigated steel [24-26]. To exclude the influence of the mesh or other numerical artifacts, all of the RVEs were meshed with six-node C3D6 elements with very fine mesh size (approximate 24000 elements) and implemented periodic boundary.

Fig. 3. Artificial microstructure model of steel AISI 1045. The green regions represent pearlite colonies, the colorful regions represent the ferrite grains with different orientations.

3. Plasticity behavior of ferrite and pearlite

3.1 Crystal plasticity model for ferrite

3.1.1 Model description

The phenomenological crystal plasticity (CP) model was employed to describe the plasticity behavior of ferrite, in which 24 slip systems from $\{110\}\langle 111 \rangle$ and $\{112\}\langle 111 \rangle$ were considered. According to Roters et al. [20], the deformation gradient F can be multiplicatively separated into elastic and plastic parts:

$$F = F_e F_p, \quad (2)$$

where F_p is the plastic deformation gradient. By introducing the plastic velocity gradient L_p , F_p can evolve as:

$$\dot{F}_p = L_p F_p, \quad (3)$$

According to Rice [27], when the dislocation slip is the only process of deformation, L_p can be calculated by the shear rates on each slip system:

$$L_p = \sum_{\alpha=1}^N \dot{\gamma}^{\alpha} m^{\alpha} \otimes n^{\alpha}, \quad (4)$$

where $\dot{\gamma}^{\alpha}$ denotes the shear rate of slip system α ; m^{α} and n^{α} are unit vectors, in which m^{α} describes the slip direction and n^{α} is related to the normal to α ; N

represents the amount of active slip systems.

In phenomenological constitutive models, the critical resolved shear stress τ_c^α , which defines the slip resistance, is usually used as the state variable for each slip system. For metallic materials, the resolved shear stress τ^α is approximated as:

$$\tau^\alpha = S \cdot (m^\alpha \otimes n^\alpha), \quad (5)$$

where S is the second Piola-Kirchhoff stress tensor. The shear rate is then expressed as a power law function of τ_c^α and τ^α :

$$\dot{\gamma}^\alpha = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{\tau_c^\alpha} \right|^{\frac{1}{m^s}} \text{sgn}(\tau^\alpha), \quad (6)$$

where $\dot{\gamma}_0$ is the reference shear rate; m^s is the strain rate sensitivity parameter. When slip occurs, hardening is the result of interactions between different slip systems. This is described by the relationship between the increment of τ_c^α on the slip system α and the hardening matrix $h_{\alpha\beta}$:

$$\dot{\tau}_c^\alpha = \sum_{\beta=1}^N h_{\alpha\beta} |\dot{\gamma}^\beta|, \quad (7)$$

The hardening matrix $h_{\alpha\beta}$ represents the strain increments on slip system α due to slip on the system β . It is defined as:

$$h_{\alpha\beta} = q_{\alpha\beta} \left[h_0 \left(1 - \frac{\tau_c^\beta}{\tau_c^s} \right)^a \right], \quad (8)$$

where $q_{\alpha\beta}$ is the anisotropic latent hardening matrix; h_0 , τ_c^s , a are slip hardening parameters. $q_{\alpha\beta}$ is set to be 1.0 for coplanar and 1.4 for other cases [20]. By integrating

Eq. (7), the hardening evolution law can be expressed as:

$$\tau_c^\alpha = \tau_0 + \int_0^t q_{\alpha\beta} \left[h_0 \left(1 - \frac{\tau_c^\beta}{\tau_c^s} \right)^a \right] |\dot{\gamma}^\beta| dt, \quad (9)$$

where τ_0 is the initial value of critical resolved shear stress. The influence of grain size

on the hardening property is described by the Hall-Petch relation:

$$\tau_0 = \tau'_0 + \frac{K}{\sqrt{d}}, \quad (10)$$

where d is the grain diameter; τ'_0 and K are fitting parameters.

3.12 Calibration of parameters in the CP model for ferrite

Most researchers employ nanoindentation tests to calibrate the CP parameters of ferrite at room temperature [11,18]. In our work, all the experiments were conducted at -196 °C and it is almost impossible to perform nanoindentation test at such low temperature. Therefore, an iterative process using virtual experiments was introduced to calibrate the remaining CP parameters of ferrite, as shown in Fig. 4. The idea was to investigate a single phase ferritic steel with a similar grain size distribution of the ferritic phase in the selected grade of AISI 1045. Consequently, a pure ferritic interstitial-free (IF) steel is used to conduct tensile tests at -196 °C to provide target stress-strain curves. Based on the microstructure information of the IF steel, an RVE of the IF steel was constructed. By implementing boundary conditions and inputting CP parameters, the simulated flow curve can be extracted which have to be mirrored by the corresponding experiment. The input CP parameters were thus iteratively adjusted until the flow curve extracted from simulation could best match the experimental data.

To generate effective flow curves in RVE simulations, the stress and strain in the RVE simulations were extracted in post-processing. The average equivalent stress $\bar{\sigma}_{RVE}$ and plastic strain $\bar{\varepsilon}_{RVE}^P$ over the whole RVE volume were calculated with the following equations:

$$\bar{\sigma}_{RVE} = \frac{\sum_{i=1}^n \bar{\sigma}_i V_i}{\sum_{i=1}^n V_i}, \quad (11)$$

$$\bar{\epsilon}_{RVE}^p = \frac{\sum_{i=1}^n \bar{\epsilon}_i^p V_i}{\sum_{i=1}^n V_i}, \quad (12)$$

where $\bar{\sigma}_i$ and $\bar{\epsilon}_i^p$ denote values of von Mises stress and equivalent plastic strain of element i in a RVE; V_i is the volume of element i ; n is the number of elements in the RVE.

Fig. 4. Flow chart for determination of CP parameters for ferrite.

The experimental flow curve of ferrite was determined from tensile tests of the pure ferritic IF steel, which has the same average grain size value (13 μ m) compared to the investigated steel. Fig. 5a shows the metallography of the steel with color etching. The etching solutions is composed of 1 g K₂S₂O₅ and 50 ml water saturated with Na₂S₂O₃. As seen, the steel is purely ferritic and Fig. 5b shows the grain size distribution of ferrite.

After analysis with a gamma distribution, the parameters α and β of Eq. (1) were calculated to be 4.08 and 3.10 respectively. After performing the Kolmogorov–Smirnov testing, it is found the value of $D_{\max}$ is 0.043, which is lower than the critical value D_{critical} of 0.079, illustrating the fitting quality is good enough. Based on the microstructural information, the $200\ \mu\text{m} \times 200\ \mu\text{m}$ RVE with only ferritic grains was generated, as shown in Fig. 6. Different colors represent various orientations of ferritic grains. The micromechanical modeling was performed by implementing uniaxial tensile periodic boundary conditions on the RVE and the average Mises stress and equivalent plastic strain over the whole RVE were extracted for the simulated flow curve. As seen in Fig. 7, the simulated flow curve agrees well with the experimental one, illustrating the effectiveness of the calibrated CP parameters for the ferrite phase, as listed in Table 2. Regarding the calibration of CP parameters, the adapted CP parameters are shown in Table 2 except that values of C_{11} , C_{12} and C_{44} were taken from reference [18]. The calibrated CP parameters might not be unique.

Fig. 5. (a) Microstructure and (b) grain size distribution of the ferritic IF steel.

Fig. 6. The artificial microstructure of the ferritic IF steel.

Fig. 7. Comparison of the simulated and experimental flow curves of the ferritic IF steel.

Table 2 Parameters of the CP model for ferrite.

C_{11}, GPa	C_{12}, GPa	C_{44}, GPa	τ'_0, MPa	$K, MPa\sqrt{\mu m}$
231.4	134.7	116.4	250	323
h_0, MPa	a	m^s	τ_c^s, MPa	$\dot{\gamma}_0, s^{-1}$
70	2.0	0.056	800	0.0001

3.2 Flow curve of pearlite

Owing to the complex structure of pearlite colonies, it is difficult to simulate the lamellar structure of cementite and ferrite. An empirical approach proposed by Allain and Bouaziz is often applied for description of the plastic behavior of pearlite in the modeling of kinematic hardening, flow behavior, fatigue and ductile failure [18, 28-

30]. According to the approach, the flow stress of pearlite is dependent on the critical lattice friction of ferrite lamella, the interlamellar spacing in pearlite and strain hardening without considering the anisotropic behavior. In these works, the isotropic flow curve can still predict results with reasonable accuracy in different studies [18, 30]. Therefore, the pearlite colony was assumed to be homogeneous in this work and the isotropic flow curve was applied to describing the plastic behavior of pearlite. A similar iterative procedure was employed to obtain the flow curve of pearlite, as shown in Fig. 8. The RVE of steel AISI 1045 was employed to perform simulation under uniaxial stress state by inputting the calibrated CP parameters of ferrite and the to-be-calibrated flow curve of pearlite. The flow curve of pearlite was iteratively optimized until the simulated and experimental flow curves were consistent with each other, as shown in Fig. 9. For the two flow curves, the "consistent" in this work means their difference of equivalent stress at same equivalent strain is less than 5%. The derived flow curve of pearlite is plotted in Fig. 10.

Fig. 8. Flow chart for determination of flow curve of pearlite in steel AISI 1045.

Fig. 9. Comparison of experimental and simulated flow curves for steel AISI 1045.

Fig. 10. The derived flow curve of pearlite in steel AISI 1045.

4. Scale bridging by virtual experiments

In our past research [10], a macromechanical model has been proposed to study the influences of plastic strain, as well as the stress state on the cleavage fracture behavior for the modern steels of excellent cleanness. The model is based on classical Orowan criterion and extends the criterion with microcrack initiation strain description. Since there are scatters for the microcrack initiation strain in cleavage fracture experiments, Weibull distribution [31] is applied to describing the scatter of the microcrack initiation strain:

$$P_f = 1 - \exp \left[- \left(\frac{\bar{\varepsilon}_{mci}^p - \varepsilon_{min}}{\varepsilon_u - \varepsilon_{min}} \right)^m \right] \quad (13)$$

where ε_u is the scale parameter of equivalent plastic strain and equal to $\bar{\varepsilon}_{mci}^p$ at $P_f = 0.632$; ε_{min} is the threshold strain value to initiate a microcrack; and m is the third Weibull distribution parameter describing the shape of the curve. With the results of different mechanical tests including tensile tests with notch round bars, plane strain specimens and three point bending tests, the microcrack initiation strain locus and parameters in Eq.(13) were calibrated.

In the study, two-dimensional RVEs with small thickness were generated to investigate the stress-state-dependent behavior of cleavage fracture, which is under plane stress condition. For such condition, the uniaxial tension, plane strain tension, and equibiaxial tension are three typical stress states for investigation [32]. Since the stress triaxiality of the macromechanical modeling calibrated is in the range of 0.6-2 [10], the plane strain and equibiaxial tension were implemented on the RVE to perform simulations in current work for comparison. Fig. 11 shows the results of RVE simulation with the same global strain under different boundary conditions. It can be seen that stress distribution in the RVE under equibiaxial and plane strain tension are totally different, which indicates a pronounced stress state effect.

Fig. 11. Simulation results of (a) the generated RVE under (b) equibiaxial tension and (c) plane strain tension ($\times 10^6$ MPa).

For the investigated steel, nucleation of microcracks has been proven to be held on cementite lamellae in pearlite [21]. The cleavage fracture includes stages of microcrack initiation and propagation. The most difficult stage of crack formation is identified as the critical stage since it controls the microscopic cracking process and defines the criteria for the occurrence of cleavage fracture behavior. The critical stage can be microcrack nucleation or propagation depending on different stress states. Since it is difficult to simulate lamellae structures in the current RVEs, the assumption that the critical stage of cleavage fracture is microcrack propagation is taken. The assumption is reasonable. This is because at very high stress triaxiality, the nucleation of microcrack is more likely to be the critical stage of cracking at -196°C . For stress states of plane strain tension and equibiaxial tension, the stress triaxialities are 0.58 and 0.67, which are lower than 0.99. Thus, microcrack propagation has large possibility to be the critical stage [21]. During the propagation, a potential microcrack from the cementite lamella extends into the surrounding ferritic phase by overcoming the resistance of interfacial boundaries. Those features were drawn aside in this part of work because no experimental proof of intervention of such barriers has been presented in the literature for the considered temperature to the authors' knowledge. Thus, the fracture propagating from a pearlite colony to other ferrite grains or pearlite colonies is assumed to be the critical stage of cleavage fracture at the investigated stress states, plane strain tension and equibiaxial tension. The resulting mechanical criterion for fracture can then be expressed as a simplified Griffith's criterion for a penny-shaped crack extension. The classical assumption of the weakest link theory is also considered for this purpose.

This means when a crack propagates through any pearlite grain, cleavage fracture occurs. According to the reference, the local fracture stress of the pearlitic steel with coarse pearlite is 1600 MPa at -196°C [33]. In this work, the average lamella spacing with 500 measurements is 0.28 μm , which is quite similar to 0.25 μm , the average lamella spacing of the reference. Therefore, the cleavage damage criterion is

$$\sigma_1^{\text{pearlite}} = \frac{\sum_{j=1}^n \sigma_1^j V_j}{\sum_{j=1}^n V_j} \geq 1600 \text{ MPa} \quad (14)$$

where $\sigma_1^{\text{pearlite}}$ is the average maximum principal stress over a pearlite grain, σ_1^j is the maximum principal stress of the element j and V_j is the volume of element j in the pearlite grains. In other words, when the average principal stress over any pearlite grain reaches 1600 MPa, cleavage fracture will be triggered.

With the generated RVE, the plasticity of each constituent and local critical criterion, virtual experiments can be conducted with different boundary conditions. In order to consider the scatter of cleavage fracture, 50 various RVEs with the statistical information (phase fraction and grain size distribution) of microstructure for steel AISI 1045 were generated. Those RVEs were further implemented under plane strain and equibiaxial conditions to perform the simulations. After simulation, the local fracture criterion is applied to extract the microcrack initiation strain $\bar{\epsilon}_{mci}^p$, which is the average plastic strain of the whole RVE ($\bar{\epsilon}_{RVE}^p$) at the moment when the local cleavage criterion is reached. Fig. 12 shows the position of the critical pearlite grain in the RVE, whose average maximum principal stress has reached 1600 MPa first.

Fig. 12. The position of pearlite that initiates the cleavage fracture under plane strain tension ($\times 10^6 \text{MPa}$); Green regions represent pearlite colonies and different color regions represent ferrite grains with different crystallite orientations.

By conducting virtual experiments with the 50 RVEs at plane strain and equibiaxial stress state respectively, 50 values of $\bar{\varepsilon}_{mci}^p$ for each stress state were extracted. The $\bar{\varepsilon}_{mci}^p$ were then ranked by the order of quantity. The probability of failure is defined as:

$$P_f^{(k)} = \frac{k - 0.3}{N + 0.4}, \quad (15)$$

where N is the total number of $\bar{\varepsilon}_{mci}^p$ and k is the sequence of $\bar{\varepsilon}_{mci}^p$. Afterwards, the distribution of $\bar{\varepsilon}_{mci}^p$ can be described by the Weibull distribution function of Eq. (13)

5. Results and discussion

5.1 Prediction of microcrack initiation strain for cleavage fracture

By conducting virtual experiments, the values of $\bar{\varepsilon}_{mci}^p$ are extracted under plane strain tension and equibiaxial tension, as shown in Fig.13. Furthermore, based on Eq. (15), the generated microstructure configurations of RVE at failure probabilities of 5, 50 and 95% under plane strain tension and biaxial tension are presented in Fig. 14 and 15 respectively, which indicate that the scatter of the cleavage fracture initiation from these multiple simulations is related to the RVEs with the same microstructural input. The Weibull distribution is applied to describe the distribution of microcrack initiation

strain. The fitted parameters of ε_u , ε_{min} and m are listed in Table 3, in which the parameters from macromechanical modeling are included as a reference. To quantify the fitting quality, Kolmogorov–Smirnov testing was performed again to check for the significance of our calibrated distribution function. The values of D_{max} are 0.11 and 0.15 for plane strain and equibiaxial tension respectively, which are both lower than the critical value of 0.19. The calibrated values of ε_{min} are both 0 for plane strain and equibiaxial tension, which agree well with the result of a corresponding macromechanical model [10]. The predicted values of ε_u are 0.055 and 0.106 for plane strain and equibiaxial tension respectively and further compared with the values calibrated by macromechanical modeling as shown in Fig. 16 [10]. Obviously, the values of ε_u by two approaches agree well with each other under both conditions. However, there is some difference between the m values calibrated by the two types of modeling.

Fig. 13. Simulated Weibull distribution of $\bar{\varepsilon}_{mci}^p$ under (a) plane strain tension and (b) equibiaxial tension.

Fig. 14. Microstructure configurations of generated RVEs at failure probabilities of 5%, 50% and 95% under plane strain tension.

Fig. 15. Microstructure configurations of generated RVEs at failure probabilities of 5%, 50% and 95% under equibiaxial tension.

Table 3 Calibrated Weibull distribution parameters at different stress states.

Method	Stress state	ε_u	m	ε_{min}
Micromechanical modeling	Plane strain tension	0.055	2.04	0
	Equibiaxial tension	0.106	1.84	0
Macromechanical modeling	Plane strain tension	0.039	4.0	0
	Equibiaxial tension	0.073	4.0	0

Fig. 16. Comparison of ε_u values of different stress states between micro- and macromechanical modeling.

To achieve a uniform comparison in terms of failure predictions, the mechanical response of unit cells is investigated with either the micromechanical or the macromechanical criteria applied. The unit cell of $1\text{mm} \times 1\text{mm} \times 1\text{mm}$ size is constructed and imposed with plane strain and equibiaxial tension boundary conditions to perform simulations. By employing the microcrack initiation strain criterion from macro and micromechanical modeling, the sudden force drop can be predicted. Fig. 17 shows the comparison of failure area within the range of 5–95% probability predicted by macro and micromechanical modeling. It can be found that the failure areas predicted by the two approaches overlap with each other and the left borders predicted by the two approaches are very close. Yet the failure area predicted by micromechanical modeling is relatively larger, indicating the scatter of cleavage fracture predicted by micromechanical modeling is larger. This is because the value of m taken from micromechanical modeling is smaller than that of macromechanical modeling. Overall, the micromechanical modeling approach can be used to predict cleavage fracture with reasonable accuracy, especially for the lower limit of the cleavage fracture initiation . On the other hand, the deviation of prediction by micromechanical modeling can be induced by the simplification of pearlite structure, assumed perfect interface between ferrite and pearlite grains in the model and the 2D RVE with a thin thickness. In the future, these factors should be considered to improve the accuracy of prediction with the micromechanical modeling.

Fig. 17. Comparison of failure within the range of 5–95% probability predicted by micro- and macromechanical modeling under (a) plane strain tension and (b) equibiaxial tension.

5.2 Microstructure sensitivity study of cleavage fracture

The presented approach can also be used to study the influence of microstructure on cleavage fracture, which is significant for material design. In this work, RVEs of two steels with pearlite fractions of 80% and 20% and the same grain size distribution of steel AISI 1045 were generated to study the effect of phase fraction on cleavage fracture. Here an implying assumption has been made that the CP parameters will not change with different volume fractions of phases which is worth to be checked. However, it still works to see the trend of plasticity and cleavage fracture with different phase fractions. The RVEs of the virtual materials and the investigated steel are shown in Fig. 8. For each virtual steel, 50 RVEs were generated and imposed with plane strain tension to perform simulations. After performing the simulation, the flow curves of steels were extracted, as shown in Fig. 9. As seen, there is a scatter of flow curves, but it is not significant, illustrating the appropriate selection of RVE size. In addition, it is also found that with increasing fraction of pearlite, the strength of the steel grows. This is because the pearlite and ferrite are hard and soft phases in the ferritic-pearlitic steel

respectively. By adding more pearlite in the RVE, the yield stress increases.

By applying the same criterion in the micromechanical modeling of the steel AISI 1045, the microcrack initiation strains are extracted for the two virtual steels, as shown in Fig. 20. The Weibull distribution was applied to describe the strain distribution of two virtual steels. The fitted parameters are shown in Table 4. After performing Kolmogorov–Smirnov testing to check for the significance of our calibrated distribution function, the values of $D_{\max}$ of the virtual material containing 80% pearlite are determined to be 0.11 and 0.074 for plane strain and equibiaxial tension condition. For the virtual material containing 20% pearlite values of $D_{\max}$ are determined to be 0.070 and 0.065 for plane strain and equibiaxial tension condition. It is found all values of $D_{\max}$ are smaller than the D_{critical} of 0.19 indicating the fitted Weibull distribution can describe the microcrack crack initiation strain data well. It can be seen that all the calibrated values of $\varepsilon_{\min}$ are 0, which are identical for the three steels. That means the threshold value of microcrack initiation strain does not change with the variation of phase fraction. In addition, the predicted m values of all steels are ~ 2 , which is also similar to the investigated steel. The predicted values of ε_u are also compared with the investigated steels, as shown in Fig. 21. It is found that the predicted ε_u values are 0.044, 0.055, 0.132 for steels with 80%, 57% and 20% fractions of pearlite phase respectively. Obviously, the ε_u grows with the decrease of pearlite fraction. This is because the $\bar{\varepsilon}_{mci}^p$ in RVE associates with the stress partitioning in different constituents of steels. When the fraction of pearlite phase increases in the steel, the ferrite fraction decreases. The stress intensifies in the pearlite colonies with less strain of the whole material, leading

to earlier microcrack initiation. On the contrary, in the RVE with 20% pearlite, most of the ferrite grains can be easily deformed and there is less stress concentration in the pearlite grains. As a result, the microcrack initiation strain decreases with the increase of pearlite fraction. Herein, the above results sufficiently identify the approach of micromechanical modeling can be used to investigate influence of ferrite fraction on cleavage fracture. Other aspects of microstructure sensitivity on cleavage fracture such as the grain size of ferrite can also be performed with the approach and shall be done in the future.

Fig. 18. RVEs with pearlite fractions of (a) 80%, (b) 57% (AISI 1045) and (c) 20%.

Fig. 19. Flow curves of different steels.

Fig. 20. Weibull distribution of microcrack initiation strain under plane strain tension for designed materials with (a) 80% pearlite and (b) 20% pearlite.

Table 4 Calibrated Weibull distribution parameters under plane strain tension.

	ε_u	m	ε_{min}
Ferrite 20%, Pearlite 80%	0.044	2.28	0
Ferrite 80%, Pearlite 20%	0.132	2.35	0

Fig. 21. Comparison of predicted values of ε_u .

6. Conclusions

This work presented an approach of micromechanical modeling to predict the cleavage fracture behavior of a steel of grade AISI 1045. The following conclusions can be drawn:

- Based on microstructure information of the steel AISI 1045, an artificial microstructure model was generated and applied in virtual experiments to study the

mechanical behavior of the material. A new method was proposed to calibrate the CP parameters of ferrite and isotropic flow curve of pearlite in the investigated steel at -196°C.

- Imposed with a local stress criterion, 50 RVEs of steel AISI 1045 were generated to perform micromechanical modeling under plane strain tension and equibiaxial tensions. The predicted microcrack initiation strains at different stress state show reasonable accuracy compared with the results of macromechanical modeling calibrated by experiments. The approach successfully upscales the cleavage damage from microscale to macroscale.
- The micromechanical approach offers an interface for the computer-aided design of microstructure. By using tailored RVEs with different fractions of microstructure constituents, the influence of phase fraction on mechanical properties and the cleavage fracture was quantitatively studied. The results indicated that with the increasing amount of pearlite, the strength of steel increases but the microcrack initiation strain decreases. The approach can be further applied to study other factors, like grain size influence on cleavage fracture for optimization of the microstructure to meet desired mechanical properties.

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Graphical abstract

Highlights:

1. A microstructure-based micromechanical modeling approach is proposed to predict cleavage fracture.
2. The crystal plasticity parameters of ferrite and isotropic flow curve of pearlite at -196°C are calibrated.
3. The approach successfully upscales the cleavage damage from microscale to macroscale.
4. The approach is applied to a microstructure sensitivity study on cleavage fracture.

Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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