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Numerical modelling of cleavage in high strength steels with parametric study on microstructures

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Abstract

One of the challenges in cleavage modelling is the strong sensitivity to material characteristics at the micro level. In this research, a microstructure-based method that is coupled with Finite Element Analysis is used to model the cleavage behavior of a S690 QT steel at -130°C. The method is a multi-barrier model which accounts for microcrack nucleation by hard inclusions and microcrack propagation based on the weakest link mechanism. In this article, parametric variations of grain size, second particle size, and second particle density are performed. This study can help inform the trade-off between microstructural parameters, and help a designer choose a process for controlling toughness. By comparing the simulations, it is found that the reduction of grain size is more effective than the reduction of brittle particle size and distribution on toughness improvement for the studied material.

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Keywords: Cleavage; Statistical modelling; Fracture toughness; Multi-barrier modelling; Local approach to fracture

1. Introduction

In order to balance cost, toughness, strength, and other performance attributes, it is critical for material designers to know the effects of various microstructural features on cleavage. Since brittle fracture is a highly localized

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phenomenon, one of the challenges in its modelling is the strong sensitivity to material characteristics at the micro level. A numerical method was proposed (Jiang et al. 2022) based on prior multi-barrier models (Martín-Meizoso et al., 1994) and has been demonstrated on fracture data from a S690 QT steel plate that was fractured at -100 ° C. The method represents the cleavage fracture toughness of steels incorporating the statistical information of microstructures and tensile properties. The method accounts for several microstructural features (grain size, hard particle size, and hard particle geometries) simultaneously, and incrementally considers the deactivation of crack initiators. It offers an opportunity to contextualize existing empirical observations (e.g. Ray et al. 1995) that relate microstructural features to cleavage. In this article, variations of microstructural parameters, such as grain size and second particle distributions, are performed (while keeping other modelling parameters constrained) in order to find the correlations with macroscopic fracture parameters.

2. Materials and models

2.1. Microstructure of the material

A S690 QT steel is used as the basis for the parametric studies presented in this article. The specimens are taken from the middle section of a 100 mm thick plate and have a mixed tempered martensitic-bainitic microstructure. Microstructure characterizations are performed with EBSD measurements as described in Bertolo (2022). From analysis of the reconstructed Prior Austenite Grains (PAG), the statistical distribution of grain size has been measured. To quantify the grain size (*D*) in cleavage modelling, least-square fitting is performed on the grain size data to get the function representing the distribution:

$$P(\text{major axis} > D) = min\left\{1 - lognormalCDF(D, \mu, S), \frac{\alpha}{D^{\beta}}\right\} \quad (1)$$

where α and β are fitting parameters, and lognormalCDF(D, μ, S) represents $1/2 + 1/2\text{erf}\,[(\ln(D) - \mu)/\sqrt{2}\,S]$, where μ is the mean and *S* is the standard deviation.
Fig. 1 (a) shows the grain size data with the fitted formula.

SEM was used to characterize the inclusions. The steel contains spherical inclusions which are mainly oxides. The density of inclusions is determined to be 7.8 per 0.001 mm^3. Eq. (1) is also used to represent the distribution of inclusion diameters (*d*).

Fig. 1 (b) shows the measured statistical distribution of spherical inclusion sizes and the fitting.

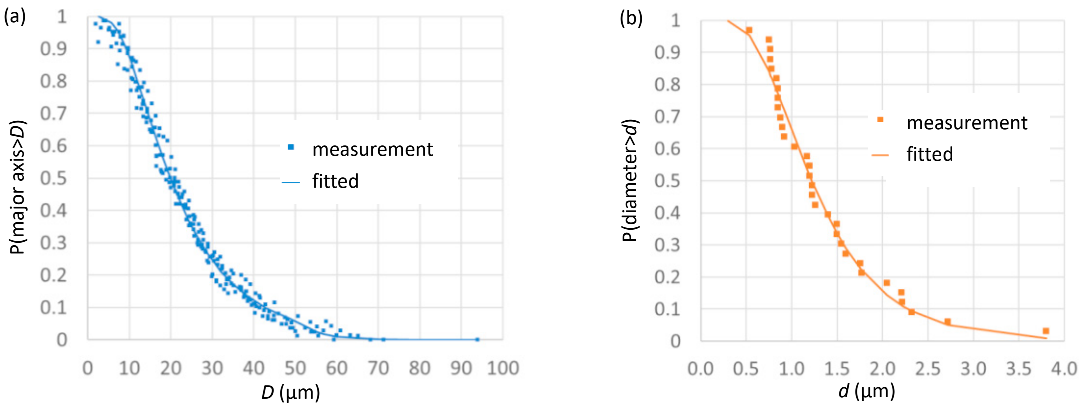

Fig. 1 Distribution of the (a) major axis of PAG (b) diameter of spherical inclusions

2.2. Finite Element model

Fracture toughness tests were performed at -130 °C according to the standard ISO 12135 (2018) using Single Edge Notched Bending (SENB) specimens, with dimensions of 20×10×92 mm^3, and crack depth to width ratio *a/W* of 0.5

and 0.25. Each specimen is modelled in Abaqus 2017 as a 3D deformable solid by using symmetry. The support and load roller are modelled as frictionless analytical rigid surfaces. The initial prefatigued crack tip is modeled as a finite notch that is 0.005 mm in radius. A 20-noded hexahedral element with reduced integration (C3D20R) is used for the mesh. The smallest element near the crack tip has a dimension of 0.001×0.005×0.067 mm^3. Displacement control is used to apply a total deflection of 1 mm. A full Newton-Raphson algorithm is used to solve the geometric and material nonlinearity in an implicit method. The stress-strain relationship of the steel is characterized by Ludwik's law, which is defined with the flow stress (σ) and the effective plastic strain (ε_p) as:

$$\sigma = \sigma_y + K\varepsilon_p^{n_L}. \tag{2}$$

where σ_y is yield stress, and K and n_L are hardening parameters. The parameters of Ludwik's law are fitted from tensile tests and are used to generate material input for the FE model. Tensile tests were carried out at -130°C according to ISO 6892-3 (2015), and the resulting values of the parameters are: Young's modulus is 236 GPa, σ_y = 888 MPa, K = 593 MPa, and n_L = 0.66. The material can be considered isotropic.

2.3. Statistical model of cleavage

The statistical model applied in this research was developed by Jiang et al. (2022) based on a multiple-barrier theory of the cleavage mechanism (Martín-Meizoso et al., 1994). The cleavage fracture of steels is regarded as the result of successive occurrence of three events:

I: nucleation of a crack at a brittle second-phase particle.

II: propagation of the microcrack across the particle/matrix interface.

III: propagation of the grain-sized crack to neighbouring grains across the grain boundary.

The stress level needed for inclusion cleavage is characterized by the critical particle strength σ_H^C. It is assumed that the value of inclusion strength is uniformly distributed in the range [σ_H^C, $\sigma_H^C + \Delta\, \sigma_H^C$]. For a volume that contains N inclusions, the number of cracked inclusions (N_{cr}) is in proportion to the inclusion stress σ_H and can be calculated as

$$N_{cr} = \min\{N \times (\sigma_H - \sigma_H^C)/\Delta\, \sigma_H^C, N\} \geq 0. \tag{3}$$

where the inclusion stress σ_H is calculated from the first principal stress of the matrix $\sigma_{1,matrix}$ and the equivalent von Mises stress of the matrix $\sigma_{eq,matrix}$, by

$$\sigma_H = \sigma_{1,matrix} + f_\alpha \sigma_{eq,matrix}, \tag{4}$$

where the factor f_α is determined using the analytical solution proposed by Jiang et al. (2021) based on the inclusion geometry.

Critical stress is usually used as a criterion for the crack propagation across the particle/matrix interface or across the grain boundary. In the present paper, the equivalent matrix toughness at the particle/matrix interface is characterized by the local cleavage parameter K_{Ia}^{pm}, and the equivalent toughness at the grain boundary is characterized by the local cleavage parameter K_{Ia}^{mm}. A minimum particle size (d_c) and a minimum grain size (D_c) are calculated for the first principal stress within the grain ($\sigma_{1,matrix}$) to propagate the micro-crack across the particle/matrix interface and grain boundary, by:

$$d_c = (K_{Ia}^{pm}/\sigma_{1,matrix})^2 \tag{5}$$

$$D_c = (K_{Ia}^{mm}/\sigma_{1,matrix})^2. \tag{6}$$

Finite element analysis (FEA) of a macroscopic volume gives the stress/strain distribution (which contain $\sigma_{1,matrix}$, $\sigma_{eq,matrix}$ values within each finite element) at each load increment. The cleavage probability is calculated from a cleavage check based on the stress level, shape of the stress field, and statistical information of the microstructure. The probability of a micro-crack propagating as cleavage fracture is based on hard particle size $d > d_c$ and grain size $D > D_c$. By accounting for the cleavage probability of all finite elements in the fracture process zone (areas that are plastically deforming), the total failure probability (P_f) of the specimen can be calculated and can be expressed as a function of the global load.

In addition to FEA stress and strain results, the required input includes f_α calculated from inclusion geometry, the distribution density function of the grain size, the distribution density function of the hard particle size, number of inclusions per elementary volume, cleavage parameters K_{Ia}^{pm}, K_{Ia}^{mm} and σ_H^C. Other parameters that need to be defined are threshold plastic strain $\varepsilon_{p,thre}$, elementary volume V_0, and scatter of the inclusion fracture strength $\Delta\,\sigma_H^C$. The predefined values are summarized in Table 1.

Table 1 Value of the input parameters

Parameters	Values
Threshold plasticity strain $\varepsilon_{p,thre}$	10^{-5}
Elementary volume V_0	0.001 mm^3
Stress factor of spherical inclusion f_α	0.239
Scatter of the inclusion fracture stress $\Delta\,\sigma_H^C$	0.10 GPa

3. Study on the effect of microstructural features

The value of K_{Ia}^{pm} (particle/matrix interface toughness) is determined from the cleavage surface analysis. The smallest inclusion that was identified as local cleavage fracture initiation site by Cheekati (2022) is of size 1.08 (±0.10) µm. The micro-cracks of these inclusion size are able to propagate across the inclusion/matrix interface and form cleavage facets among neighbouring grains. FEA shows the $\sigma_{1,matrix}$ is 2.6 GPa at the location of crack initiation site. K_{Ia}^{pm} is calculated as 2.7 MPa√m with the identified particle size and stress level using eq. (5). Cleavage parameters K_{Ia}^{mm} (grain boundary toughness) and σ_H^C (brittle inclusion strength) are determined by inverse analysis (maximum likelihood fitting) from the measured CTOD. The fitting data include 9 deep cracked (*a/W*=0.5) and 15 shallow cracked (*a/W*= 0.25) specimens. All specimens that were used are fractured at -130°C and have a brittle fracture mode. Fig. 2 shows the comparison of experiments and the simulation using the fitted parameters K_{Ia}^{mm} = 22.8 MPa√m and σ_H^C = 2.9 GPa. It shows that the fitted parameters can represent the statistical distribution of CTOD and reflect the influence of initial crack depth (*a/W*).

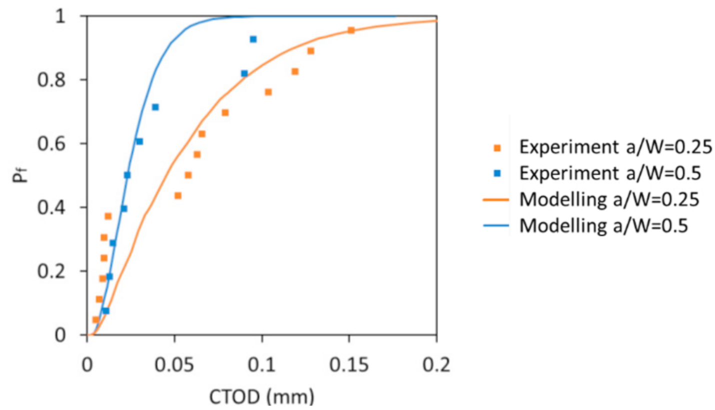

Fig. 2 Cleavage probability calculation of the S690 QT steel based on fitted parameters

The microstructures of high strength steel can be optimized in three ways to improve the toughness while yield strength is preserved: by refining the grain size, by refining the brittle particles, and by reducing the density of brittle particles. Parametric simulations are performed, assuming grain sizes, particle size, and particle density are changed independently. The simulations are performed with cleavage parameters determined from the as-received material (K_{Ia}^{mm} = 22.8 MPa√m and σ_H^C = 2.9 GPa). Another simulation is performed for increased flow stress as it can be a consequence of the refined grain size. Because the degree of correlation among grain size, particle size, amount of brittle particles, and flow stress varies in different materials, it is essential to quantify the degree of importance of each factor separately. Fig. 3 shows the sensitivity of normalized CTOD values to each of the material factors. The reduction of grain size is more effective than the reduction of brittle particles or the refining of particle size on toughness improvement. Although the increased yield stress shows a detrimental effect on toughness, this influence is much less than the improvement effect of refined grain size, especially considering that the correlation between grain size and yield strength is a Hall-Petch relationship:

$$\sigma = \sigma_0 + k_y D^{-1/2} \tag{7}$$

where σ_0 is the starting stress for dislocation movement, k_y is the strengthening coefficient, and *D* is the grain size.

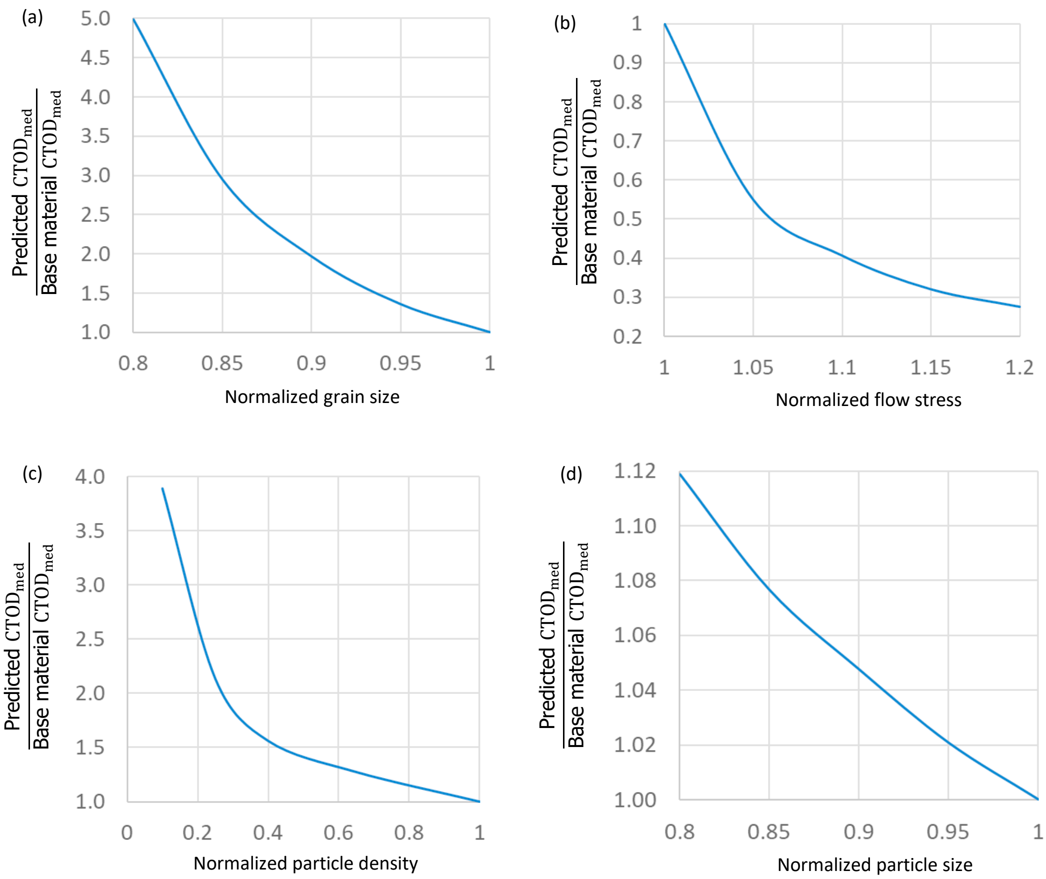

Fig. 3 Simulated median CTOD values of varied material factors (a) reduced PAG size (b) increased flow stress (c) reduced particle density (d) reduced particle size

The study indicates that the grain size is the most dominant factor although particle size distribution does show a distinct effect. It can be explained that the brittle particles in the studied material are inclusions of relatively large size (above micrometer) compared to the minimum size of microcrack that can propagate across the particle/matrix interface. The critical grain size defined by eq. (6) is in the tail of the coarse grains. Slight grain refinement leads to a large reduction of the number of microcracks that can propagate across the grain boundaries.

4. Conclusion

By comparing the simulations of parametric variations on grain size and second particle distributions of S690 QT steel, the effects of microstructural parameters for controlling toughness are quantitively estimated. The following conclusions are highlighted:

- The multi-barrier method quantitively captures the effect of multiple microstructures on fracture toughness.
- The reduction of grain size is more effective than the reduction of brittle particle size for improving toughness for the studied material.
- The more dominant influence of grain can be explained by the relative relationship between microstructure's size distributions and crack-resistance of microstructure's boundaries.

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