Prediction of fracture behavior in hole expansion test using microstructure based dual-scale model

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Abstract. A reliable prediction of sheet formability is required for designing automobile parts, especially for the parts made of Advanced High Strength Steels (AHSS) with complex microstructure. Because of the microstructural complexity of AHSS, finite element (FE) simulations based on the representative volume element (RVE) in which microstructural information is incorporated as a submodel have been used to predict macroscopic mechanical properties of materials. In this work, a dual-scale FE approach was proposed to predict the hole expansion ratio (HER) of a multiphase steel sheet. As a large scale simulation, punching analysis followed by the hole expansion simulation was first performed. The strain history of each element was used as a boundary condition for the subsequent small-scale RVE model. Deformation behavior depends on several factors related to microstructural effects such as grain size, and dislocation density. The equilibrium dislocation density in the pile-up configuration was calculated by applying the Peach-Kohler equation and the mean free path was calculated from the derived dislocation density. The dislocation density based flow stress was implemented in the model. For the failure modeling, realistic microstructure-based finite element approach was presented in combination with continuum damage mechanics to consider the microstructure of investigated steel. In the simulation of punching process, a ductile fracture criterion was suggested to predict shear and fracture zones. The experimentally observed hole-expansion formability was reasonably explained by using the presented dual-scale finite element model.

1. Introduction

The prediction of ductile fracture in the advanced high strength steels (AHSS) has been challenges in automotive industries due to their complexity in microstructures. Numerous studies tried to predict accurate fracture behavior using various constitutive models [1-3]. Most of the works used damage variables to take into account the deterioration of materials from the continuum aspect. For example, Johnson and Cook [4], as one of representative fracture models, introduced cumulative strain as a damage indicator. An alternative approach to the continuum based fracture models is to use micromechanical characteristics of ductile metals. The microstructure based model proposed by Needleman and Tvergaard [5] falls in this category and they introduced a void volume fraction to measure the material’s deterioration by the void growth and coalescence under different stress states.
The use of representative volume element (RVE) to model microstructure and to investigate the formation of microcracks under the various loading conditions is a prospective way to predict the fracture behavior of the AHSS [6, 7].

In this work, various fracture criteria were evaluated using the realistic microstructure based dual-scale finite element approach. Deformation history from macroscale simulation was used as a boundary condition for microscale simulation. The flow behavior of 780HB was modelled using dislocation based constitutive equation. The mechanical properties calculated form microscale simulation were used as a function variables to predict equivalent fracture strain. Material parameters for each criterion were optimized using uniaxial tensile test and notched tensile test.

2. Experiments

2.1. Material

780 grade high burring hot-rolled steel (780HB) with a ferrite single phase was used. The high burring steel is featured by its large elongation and hole expansion ratio. Figure 1a shows the microstructure of 780HB identified by electron backscatter diffraction (EBSD). The step size was 50 nm and the average grain size was 5μm with the misorientation angle of 5 degrees. From the image quality (IQ) map, both polygonal and acicular ferrite were observed. Since the investigated steel was hot-rolled, no preferred orientation was found from the inverse pole figure (IPF) map. Mechanical properties were obtained from uniaxial tensile test with strain rate of 0.001/s and the stress-strain curve is shown in figure 1b.

\[ \sigma = k (\varepsilon_0 + \varepsilon)^n \]

Figure 1. (a) EBSD image. IQ map (left) and IPF map (right). (b) stress – strain curve.

2.2. Hole expansion test

Sheet samples with a circular hole (with a diameter of 10mm) at the center of specimen were prepared for 780HB sheet. Both punched and wire cut holes were considered to study the hardening effect near the hole edge. The thickness of sheet samples was 3 mm and dimension of sample was 50mm X 50mm. A conical punch with an angle of 60° moved upward with a speed of 8 mm/min and the experiments were terminated when the crack propagates throughout the top and bottom of the sample.

3. Finite element modeling

3.1. Macroscale simulation

Three-dimensional elasto-plastic FE simulation of punching and hole expansion test were conducted for 780HB. The Swift hardening model was used for the macroscale simulation.
Optimized parameters for 780HB were 1138.9 MPa, 3.429E-9, 0.1322 for \( k \), \( \varepsilon_0 \) and \( n \), respectively.

Geometric parts of simulation for punching and hole expansion are represented in figure 2a and 2b, respectively. The tip, upper and lower dies were considered as rigid body. For the sheet specimen, 8 node linear hexahedral type elements with a reduced integration were used for computational efficiency. The Coulomb friction was assumed between rigid tools and deformable specimen and the friction coefficient was set to 0.2.

![Figure 2](image)

**Figure 2.** Geometric part for finite element simulation. (a) punching, (b) hole expansion test.

### 3.2. Microscale simulation

In the microscale simulation, 3D RVE was used to consider the microstructure of investigated steel. The RVE was constructed using the grain boundary map from the EBSD data. The dimension of the RVE was 19.6 \( \mu \)m x 20 \( \mu \)m with the thickness of 0.5 \( \mu \)m and a columnar structure to the normal direction was assumed. The finite element mesh for the microscale simulation is shown in figure 3c. The total number of nodes and elements are 119968 and 89703, respectively. The element size near the grain boundary was approximately 50–100 nm.

![Figure 3](image)

**Figure 3.** Microstructure image used for finite element analysis. (a) IPF map (b) grain boundary map and (c) mesh generated from microstructure image.

#### 3.2.1. Constitutive equation

Isotropic von Mises elasto-plasticity was adopted for the microscale simulation. To define the flow behaviour of 780HB, a dislocation based flow model [8, 9] was used.
\[ \sigma = \sigma_0 + \alpha \cdot M \cdot \mu \cdot \sqrt{b} \cdot \left( \frac{1 - \exp(-M \cdot k \cdot e)}{k \cdot L_m} \right)^2 \]  
(2)

\[ \sigma_0 = 77 + 750 \cdot \text{wt}\%P + 60 \cdot \text{wt}\%Si + 80 \cdot \text{wt}\%Cu + 45 \cdot \text{wt}\%Ni + 60 \cdot \text{wt}\%Cr + 80 \cdot \text{wt}\%Mn + 11 \cdot \text{wt}\%Mo + 5000 \cdot \text{wt}\%N + 5000 \cdot \text{wt}\%C \]  
(3)

where \( \alpha \) is a constant having a value of 0.33, \( M \) is the Taylor factor (\( M = 3 \)), \( \mu \) is the shear modulus (\( \mu = 80\text{GPa} \)), and \( b \) is the Burger’s vector (\( b = 2.5 \times 10^{-10} \)). \( L \) is the dislocation mean free path and \( k \) is the recovery rate (\( k = 2 \)). The dislocation mean free path was calculated using the dislocation density derived from the dislocation pile-up theory. The relation between dislocation density and the mean free path is given as

\[ L_m = A \cdot \left( \frac{1}{\rho} \right)^{1/2} \]  
(4)

where \( A \) is a material parameter to be optimized. \( \sigma_0 \) is the contribution of the lattice friction and the elements in solid solution.

3.2.2. Dislocation pile-ups

Dislocation density developed under external stress was calculated from the 1D dislocation pile-up model. The exact dislocation density is calculated by enforcing the equilibrium condition in which the Peach-Köhler force vanishes throughout the pile-up [10].

\[ 0 = \frac{\mu b}{2n(1-\nu)}PV \left( \int_0^1 \frac{n(x')dx'}{x-x'} \right) + \sigma_A \]  
(5)

where PV indicates the principal value of the integral, \( n(x) \) is the dislocation density, \( \nu \) is Poisson’s ratio and \( \sigma_A \) is a resolved shear stress. \( D \) is a distance between dislocation source and grain boundary and \( \beta \) is the termination point of pile-up given as

\[ \beta = \left( \frac{\sigma_c}{\sigma_A} \right)^2 D \]  
(6)

In the above equation, \( \sigma_c \) is the dislocation source activation stress and is given as

\[ \sigma_c = \frac{1.2\mu b}{4\pi L_d} \cdot \ln \left( \frac{L_d}{r_c} \right) \]  
(7)

where \( r_c \) is a core radius of dislocation line and assumed to be \( 3b \). \( L_d \) is a dislocation source length, which was obtained from the TEM observation. The average value of dislocation source length was approximately 13 nm.

From the eq. (5), the resulting density is [11]

\[ n(x) = \frac{2\sigma_A (x-\beta)^{1/2}}{\mu b (D-x)^{1/2}} \]  
(8)

The dislocation density derived from the dislocation pile-up theory is a number density and this value needs to be calibrated by introducing a material parameter \( p \).

\[ \rho = n(x)^p \]  
(9)

The uniaxial tensile test with the RVE model was simulated for parameter optimization. The optimized values of \( A \) and \( p \) were 60 and 1.8, respectively. The contour map of dislocation density, von Mises stress, logarithmic strain were shown in figure 4. These constants and parameters were used for hole expansion test simulation.
3.2.3. Fracture criteria
Numerous attempts have been made to predict the fracture of materials using macroscopic variables such as a major principal stress and stress triaxiality. As the simplest criterion, the equivalent plastic strain $\bar{\varepsilon}$ is used for the fracture indicator in which failure occurs when $\bar{\varepsilon} = \bar{\varepsilon}_f$. From the uniaxial tensile test and simulation, the equivalent fracture strain was identified as 1.25. Cockroft and Latham [12] observed that fracture occurs when the accumulated value of equivalent strain multiplied by the maximum principal stress reaches a critical value. Clift et al. [13] carried out deformation test for an aluminum alloy under plain strain condition and found that the fracture occurred when the total plastic work reached a critical value.

In this study, a new ductile fracture criterion was suggested using local stress triaxiality. According to this criterion, the critical equivalent fracture strain is a function of the local stress triaxiality and expressed as

$$\bar{\varepsilon}_f = B_1 \cdot \exp(-B_2 \cdot \eta), \quad \eta = \frac{\sigma_m}{\sigma_e}$$

where $\eta$ is a stress triaxiality which is a ratio of mean stress $\sigma_m$ to the effective stress $\sigma_e$, and $B_1, B_2$ are material constants. For parameter optimization, a notched tensile test with a notch radius of 2 mm was conducted and the calibrated values were 5.404 and -3.45 for $B_1$ and $B_2$ respectively.

4. Results and discussion

**Figure 4.** Contour map under the strain of 0.12. (a) dislocation density, (b) von Mises stress, (c) logarithmic strain.

**Figure 5.** Predicted and experimental hole expansion ratio from various fracture criterion. (a) HER with wire cut sample, (b) HER with punched sample.
The strain history of the large scale simulation was imposed as the boundary condition of the lower scale RVE model. The hole expansion ratio of 780HB was predicted by applying the ductile fracture criteria. The predicted HER values by different fracture criteria are presented in figure 5. The predicted HER values from the proposed fracture criterion based on local stress triaxiality well matched with experimentally measured values, whereas the conventional criteria overestimated the experimental HER values.

5. Conclusion

Hole expansion ratio of 780HB was investigated by using realistic microstructure based dual-scale simulation and various fracture criteria. For calibration of the parameters used for each criterion, uniaxial tensile test and notched tensile test were conducted. Hole expansion tests for the samples with the punched and wire cut hole were performed to consider the edge hardening effects on punching process. In microscopic simulation, representative volume element was used to consider the microstructural properties of investigated steel on fracture behavior. The mechanical properties of constituent phase of 780HB were modelled using dislocation based constitutive equation. The strain histories of each element on macroscale simulation were used as a boundary condition of RVE simulation. A new fracture criterion was suggested using local stress triaxiality and compared with conventional fracture criteria. The results show that the suggested fracture criterion provide reasonable prediction of HER whereas the conventional criterion overestimate the HER comparing with experimental values.

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