3D-Simulation of Ductile Cracking in Two-Phase Structural Steel with Heterogeneous Microstructure

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Abstract. The effort of this study is to develop a simulation method to predict the effect of micro-structural morphology in two-phase steel, Ferrite-Pearlite steel, on structural performance in terms of ductile cracking resistance. This is based on the clarification of a *damage mechanism* to control the ductile cracking with focusing on the heterogeneity in strength of microstructure. The large number of micro-voids nucleation at lower strength side near two-phase boundary associated with the localization of stress/strain is found to control ductile cracking. According to this experimental result, we develop meso-scale 3D-model to reproduce micro-structural morphology of practical two-phase steel of interest for analyzing the stress/strain localization behaviors associated with heterogeneity of structure. Moreover, damage evolution model including the plastic potential to nucleate micro-void is proposed, so that ductile crack nucleation and subsequent growth and linking could be simulated.

The ductile cracking behavior for two-phase structural steel is simulated by means of developed meso-scale 3D micro-structural FE-model together with damage evolution model. The effect of applied triaxial stress state on critical macro-strain for ductile cracking as well as damage evolution behavior, in which critical strain could be decreased with increasing stress triaxiality, is numerically predicted.

Introduction

Ductile cracking sometimes precedes unstable fracture in brittle manner in steel structure and ductile failure under manufacturing process associated with large plastic straining. Generally, such fracture process is prone to occur under complicated history of straining with various triaxial stress states that influences critical load for ductile cracking. There have been damage models to simulate and evaluate critical load for ductile cracking of steel structures [1-5]. Most of these simulation methods are based on the homogeneous and continuous mechanics that can only be taken into account a basic and common understanding of the process of ductile cracking; nucleation, growth and coalescence of voids associated with large inclusions or second phase particles, especially the growth process, can control ductile cracking.

On the other hands, recent and future-focused structural steels have microstructural heterogeneity in strength with few large inclusions, which is dual- or multi-phase steel. One of the authors revealed that the ductile cracking controlling damage for the two-phase Ferrite-Pearlite steel could not be nucleation and growth of voids originated from large inclusions, but formation of particular number of micro-voids near the Ferrite-Pearlite boundary just before final failure [6,7]. It was found that the strength heterogeneity between crystal grains with different phases could affect ductile cracking behavior through difference in stress/strain localization behaviors.

This study proposes a simulation method for predicting the effect of micro-structural morphology on ductile cracking for two-phase structural steel on the basis of the micro-mechanism for ductile cracking through the following developments; one is 3D meso-scale FE-model that enables the analysis of stress/strain localization behaviors dependent on the morphology of two phases with strength heterogeneity in real steel, another is damage evolution and subsequent micro-void nucleation model. Comparing the experimental and simulated ductile properties as well as damage evolution in terms of micro-voids formation, the applicability of this method is validated.

Experiment of Ductile Cracking Behaviors

Experiment. The structural steel JIS SM490YB with Ferrite-Pearlite two phases with different strength in Vickers hardness (F-P steel) was used, as shown the microstructures in Fig. 1 [6,7]. Table 1 shows the chemical composition of the steel, and Table 2 lists its mechanical properties. The strength expressed by Vickers hardness of the Pearlite phase is averagely 1.4 times larger than that of the Ferrite phase. Area fraction of the hard Pearlite phase is roughly 30%.

The ductile cracking tests were conducted under single tensile loading for flat micro-tensile specimens with/without side notch in order to compare the ductile cracking behaviors under different triaxial stress state during loading. In addition, the damage behaviors in terms of voids nucleation and growth in the specimens up to ductile cracking were examined taking notice of the heterogeneous microstructures. Figure 2 shows the configuration of the employed micro-tensile specimens. The flat smooth specimens with different net-section (0.4 mm x 0.3 mm and 0.2 mm x 0.2 mm) were prepared. The side notched specimen has notch with radius of notch-root curvature *R* of 0.1 mm (R0.1 specimens), which would provide higher stress triaxiality in the middle of net-section than smooth specimens. The gage-length for measuring the tensile displacement of all specimens is 1 mm.

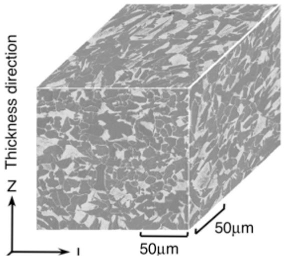

Fig. 1 Microstructures of SM490YB steel (F-P steel).

Table 1 Chemical composition of steel used.

Chemical composition (%)											
C	Si	Mn	P	S	Cu	Ni	Cr	Mo	V	B	Ceq
0.17	0.33	1.37	0.018	0.018	0.01	0.07	0.06	0.008	0.002	0.0001	0.43

C_{eq}=C+Mn/6+Si/24+Ni/40+Cr/5+Mo/4+V/14

Table 2 Mechanical properties of steel used.

Mechanical properties						
σ_Y (MPa)	σ_T (MPa)	YR (%)	ε_T (%)	El. (%)	H_V	
					Ferrite	Pearlite
344	540	64	17.6	31	198	276

σ_Y : Lower yield stress, σ_T : Tensile strength, YR : σ_Y/σ_T,
ε_T : Uniform elongation, El. : Elongation (G.L.=36mm, Dia.=6mm) ,
H_V : Average Vickers hardness (Load : 25g)

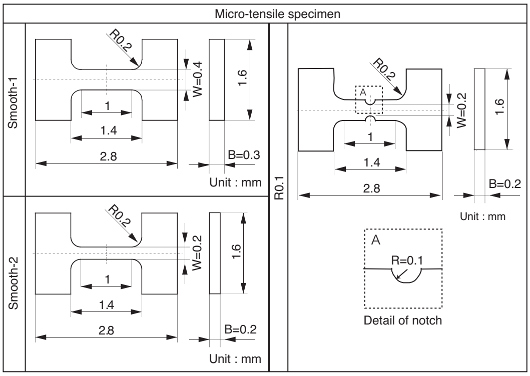

Fig. 2 Configuration of micro-tensile specimens used.

Ductile Cracking Process. The damage evolution, that is voids nucleation and growth behaviors, up to ductile crack nucleation was observed in detail by conducting tension tests for round-bar specimens with/without circumferential notch [6,7]. Until applying a large scale straining just before ductile cracking, no remarkable micro-voids were detected. After that, a particular number of micro-voids, whose size is about 1μm, and in some parts micro-voids induced micro-cracks were observed mostly at the softer Ferrite side near the Ferrite-Pearlite boundary. Finally, the ductile cracking was found to form by unstable shear fracture between these micro-voids or micro-cracks in Ferrite, in Pearlite or along Pearlite phase. These behaviors were observed irrespective of the triaxial stress state during loading. Consequently, the main controlling factor for ductile cracking in the employed two-phase steel was found to be not growth of voids induced by larger inclusions, but formation of the particular number of micro-voids just before cracking mainly at Ferrite side near the Ferrite-Pearlite boundary followed by shear fracture between them. These micro-voids formation and subsequent cracking would be caused by stress/strain localization due to heterogeneous microstructure and further localization behaviors between micro-voids.

The similar ductile cracking behaviors were confirmed in the middle of the minimum cross-section even for micro-tensile specimens used in this study. As presented for the case of Smooth-2 specimens in Fig. 3, the micro-voids and micro-cracks mainly nucleated at Ferrite side near the Ferrite-Pearlite boundary are observed only after a large amount of plastic straining.

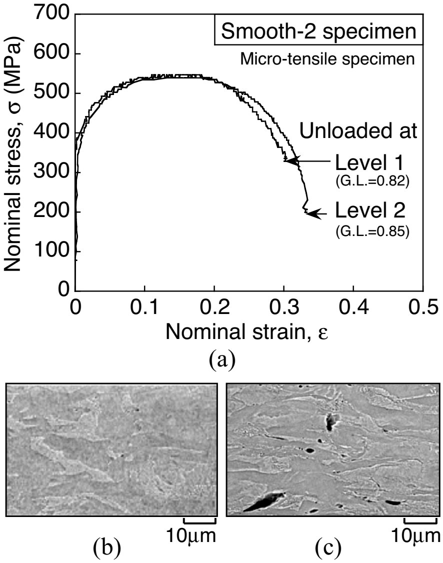

Fig. 3 Ductile cracking behaviors for Smooth-2 micro-tensile specimens, (a) s-e curves, (b) (c) SEM micro-graphs in the middle of necked section at level 1 and level 2 load, respectively.

Meso-Scale FE-Model and Damage Model for Simulating Ductile Cracking

In an effort to simulate ductile cracking of two-phase steel, the method for creating meso-scale FE-model and damage model that can simulate micro-voids nucleation and voids interaction influenced by the morphology of heterogeneous microstructure in real two-phase steel was developed.

Meso-Scale FE-model. It appears to be necessary to use heterogeneous polycrystalline model that reflect more accurate random morphology of polycrystal grains of two-phase steel, that is volume fraction, size, shape and spatial distribution of two phases, for simulating stress/strain localization behaviors. The Voronoi tessellation method [8] was applied, which can be interpreted in terms of a simple isotropic crystal growth process. Figure 4 provides the developed method for creating 3D twp-phase polycrystalline FE-model [9]. All crystalline nuclei were assumed to appear at the same instance of time, and were distributed in a space of target volume V

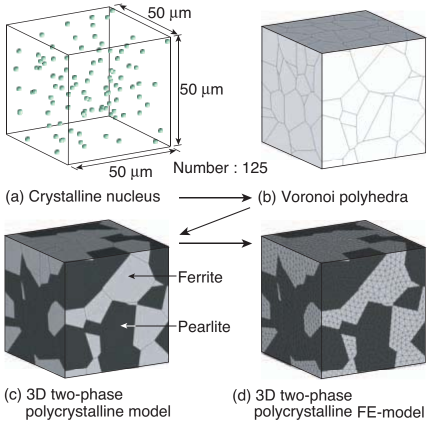

Fig. 4 Method for creating 3D two-phase polycrystalline FE-model.

(50μm x 50μm x 50μm) by random numbers (a). The polycrystal grains, that is Voronoi polyhedra, were computationally constructed as follows; for each nucleus, grain growth occurs at the same rate in all the direction (i.e. isotropic growth), and growth ceases for each cell whenever it comes into contact with a neighboring cell (b). Thereafter, the second phases were selected by generating random numbers in accordance with the practical volume fraction of second phase for two-phase steel used (i.e. in this case about 30% volume fraction of Pearlite phase) (c). Finally, the 4-node tetrahedral FE-mesh was automatically generated in this two-phase polycrystalline model (d). Figure 5 shows one example of the created 3D two-phase polycrystalline steel plate using the developed method.

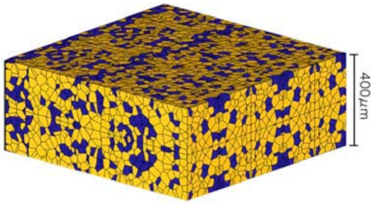

Fig. 5 Example of 3D steel plate model with two-phase polycrystal grains generated by the developed method.

Damage model. In order to simulate the micro-voids formation and subsequent these interaction behaviors that control the ductile cracking by means of developed two-phase polycrystalline FE-model, the following continuous damage model for micro-voids formation coupled with flow stress was proposed as illustrated in Fig. 6. The unit cell was assumed, where the micro-voids formation along with the flow stress of material having the damage related to random size of nano/sub-micron scale voids can be homogenized. The damage in the homogenized unit cell was assumed to be expressed by damage fraction D, where the damage increment in the unit cell was related with the increment of plastic component of volumetric strain $dE_{\mathrm{m}}^{\mathrm{p}}$ as follows.

$$dD = (1 - D)dE_{\mathrm{m}}^{\mathrm{p}} \tag{1}$$

The yield function, that is the plastic potential, of the unit cell as a function of the damage variable was proposed [10] and given as

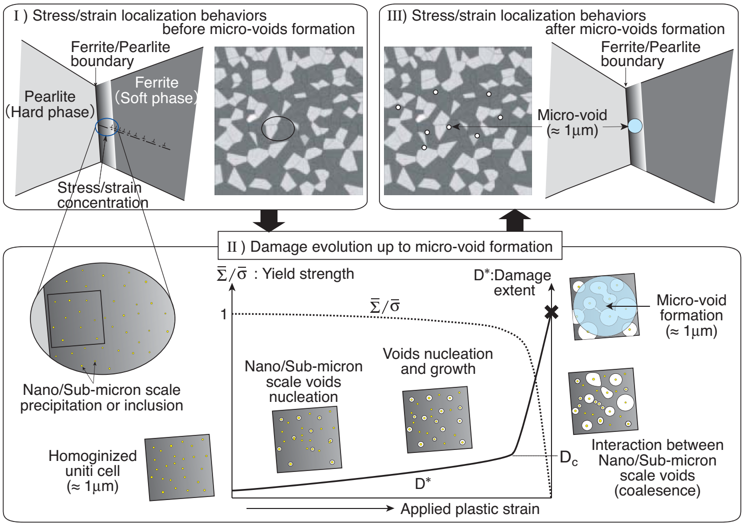

Fig. 6 Proposed damage model for simulating micro-voids formation in two-phase steel.

$$\Phi = \left(\frac{\bar{\Sigma}}{\bar{\sigma}}\right)^2 + a_1 D^* \exp\left(a_2 \frac{\Sigma_{\mathrm{m}}}{\bar{\sigma}}\right) - 1 = 0 \qquad (2)$$

where $\bar{\Sigma}$ and Σ_{m} are macroscopic equivalent stress and hydrostatic stress of the unit cell, respectively, and $\bar{\sigma}$ is flow stress of the matrix material. The parameter D^* in equation (2), which is defined in equation (3), was introduced as an effective damage parameter to take into account the loss of load carrying capacity through the parameter K [11] due to the acceleration of damage evolution after reaching the critical damage fraction D_{c}.

$$D^* = \begin{cases} D & \text{for } D \le D_{\mathrm{c}} \\ D_{\mathrm{c}} + K(D - D_{\mathrm{c}}) & \text{for } D > D_{\mathrm{c}} \end{cases} \qquad (3)$$

In the proposed yield function of equation (2), only the parameters a_1 and a_2 are the material constants to be identified.

Simulation of Ductile Cracking Behaviors

The developed two-phase polycrystalline FE-model and damage model was applied for simulating micro-voids formation and subsequent interaction induced ductile cracking.

Simulation model and parameters set. Fig. 7 shows the FE-model of R0.1 micro-tensile specimen, in which two-phase polycrystalline model was employed only around the net-section for the sake of computation time reduction. The two-phase polycrystalline model has totally 187 grains and volume fraction of hard Pearlite phase of about 30%. Average grain size is about 25µm, which is more or less larger than that for practical grain size, and element size 5µm. The stress-strain curve used for FE-analysis for homogeneous model was obtained with round-bar tensile test, and that for Ferrite and Pearlite phase was estimated from each Vickers hardness in accordance with a rule of mixture. Figure 8 shows the equivalent stress $\bar{\sigma}$ – equivalent plastic strain $\bar{\varepsilon}_{\mathrm{p}}$ curves for matrix material of Ferrite and Pearlite phases along with that obtained with tension test for two-phase steel used.

The material parameters concerning damage evolution a_1 and a_2 can be identified as follows. According to the proposed plastic potential in eq. (2), the critical strain $(\bar{E}_{\mathrm{p}})_{\mathrm{i}}$ for micro-voids formation can be expressed by equation (4) as a function of stress triaxiality [10], which includes the material parameters a_1 and a_2. Then, the test results of the stress triaxiality dependence on critical strain $(\bar{E}_{\mathrm{p}})_{\mathrm{i}}$ obtained with round-bar specimens

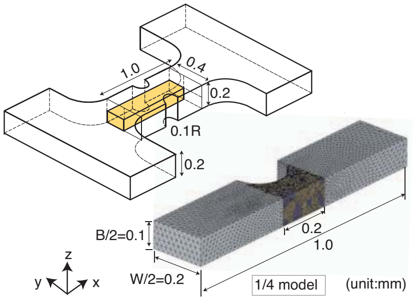

Fig. 7 3D FE-model of R0.1 specimen extracted from two-phase polycrystalline plate.

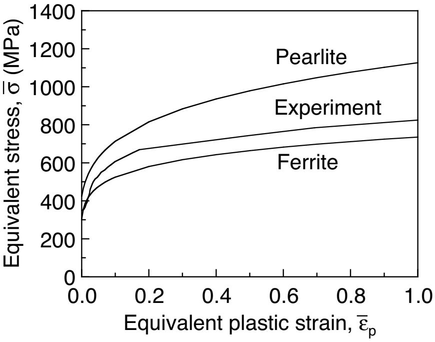

Fig. 8 Equivalent stress – equivalent plastic strain curves for Ferrite and Pearlite phases used for FE-analysis.

with/without circumferential notch directly provide damage parameters a_1 and a_2 [10].

$$(\bar{E}_{\rm p})_{\rm i} = A\exp\left(B\frac{\Sigma_m}{\bar{\Sigma}}\bigg|_{\rm const.}\right), \text{ where } \begin{cases} A = \dfrac{2}{a_1 a_2}\ln\dfrac{(1-D_0)D_{\rm c}}{(1-D_{\rm c})D_0} \\ B = -a_2 \end{cases} \tag{4}$$

In this work, these parameters for Ferrite and Pearlite phases should be determined. The parameters for each phase could be determined in accordance with the proposed procedure by manufacturing a full Ferrite and a full Pearlite steels having the same morphological and metallurgical properties as those of each phases in two-phase steel used. However, the parameters for each phase were set to be the values presented in Fig. 9 under the following assumption. The critical strain $(\bar{E}_{\rm p})_{\rm i}$ for the Ferrite phase would be much higher than that for the two-phase steel (F-P steel) obtained with circumferentially notched round-bar tension tests. Then, the $(\bar{E}_{\rm p})_{\rm i}$ at stress triaxiality of 1.2 for the Ferrite phase are assumed to be about 1.4 times higher than that for the two-phase steel obtained with tensile testing for circumferentially notched round-bar specimens with notch-root radius of 2.0 [6]. The multiplier factor of 1.4, which corresponds to the ratio of the Vickers hardness of Pearlite phase to that of Ferrite phase, was employed in accordance with the reference [12]. The stress triaxiality dependence of $(\bar{E}_{\rm p})_{\rm i}$ was also assumed to decrease with increasing volume fraction of Ferrite in steel [12]. The parameter sets for the Pearlite phase was assumed to be the same as those for F-P steel as shown in Fig. 9.

	a_1	a_2	A	B
Ferrite	1.69	1.06	2.57	1.06
Pearlite	1.09	1.48	2.84	1.48

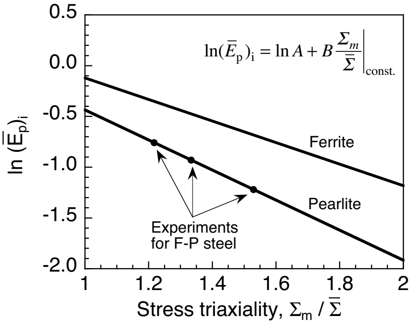

Fig. 9 Damage parameter sets for the Ferrite and Pearlite phases in two-phase steel (F-P steel) used.

The other parameters D_0 (initial damage fraction) and D_c were set to sufficiently small value of 0.0001 and 0.001, respectively, so as not to provide the loss of flow stress. The parameter K was set to a large value of 4 for both phases to accelerate the damage evolution at the last stage of micro-void formation.

The FE-analysis based simulation was conducted using ABAQUS Ver.6.4, in which a special user-subroutine for the proposed damage model was implemented referring to [13].

Results. Simulated results are compared with experimental results. Figure 10 shows relationship between nominal stress in net-section and applied strain (G.L.≈1.0mm) up to ductile cracking simulated with 3D FE-model together with the experimental results for R0.1 micro-tensile specimens. Simulated curve is in good agreement with experimental results, whereas a slight difference can be seen in the applied load range from net-section yielding to maximum stress.

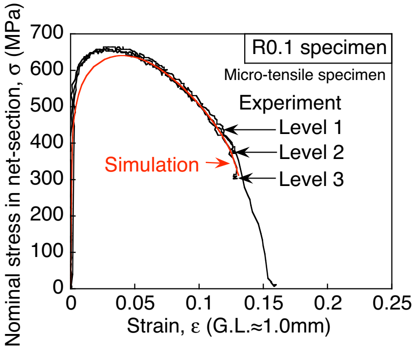

Fig. 10 Stress-strain curves for R0.1 micro-tensile specimen obtained with simulation and experiments.

Figure 11 compares the ductile damage evolution behaviors obtained with tensile tests and simulations for R0.1 micro-tensile specimens. The levels 1 to 3 in Fig. 11correspond to the applied strain levels presented in Fig. 10. The micro-voids nucleation and the ductile cracking behaviors, where the damage evolved mainly at Ferrite side at Ferrite-Pearlite boundary resulting from stress/strain localization in Ferrite, seemed to be well simulated.

The grain size modeled in the 3D polycrystalline FE-model and method for identifying the material parameters for each phase of two-phase steel need to be improved, however the proposed simulation model could be useful in estimating the effect of morphology of heterogeneous microstructures on ductile properties for two-phase steels.

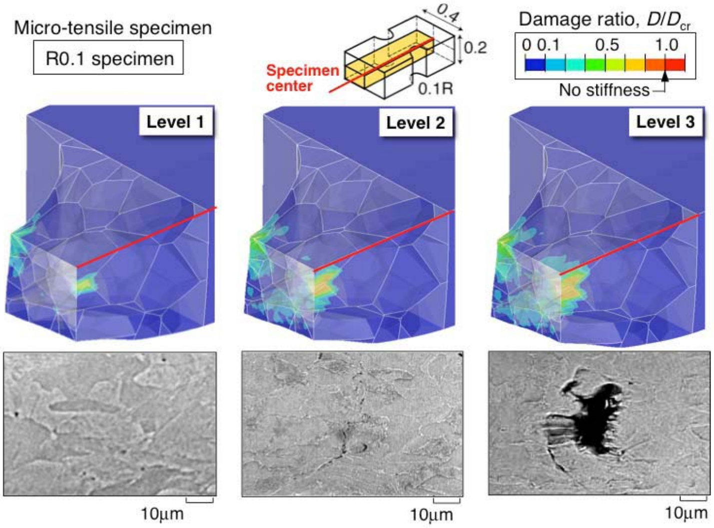

Fig. 11 Comparison between ductile damage evolution behaviors observed in experiments and simulation for R0.1 specimen.

Summary

The main controlling behavior for ductile cracking in the employed two-phase steel was found to be formation of the particular number of micro-voids just before cracking mainly at Ferrite side near the Ferrite-Pearlite boundary followed by shear fracture between them. The developed two-phase polycrystalline FE-model along with the damage model for micro-voids nucleation accounted for these micro-mechanism demonstrated that the critical strain and ductile cracking behaviors dependent on the applied triaxial stress was well simulated. The proposed method may also be useful in studying the effects of morphology of heterogeneous microstructures as well as stress triaxiality on ductile cracking properties of two-phase steels.

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