Hierarchical Damage Simulation to Correlate Micro-structural Characteristics of Steel with Ductile Crack Growth Resistance of Component

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Abstract The final goal of this study is to develop a method for estimating the effect of micro-structural characteristics of steel (especially two-phase steel) on ductile crack growth resistance of a structural component. For this purpose, hierarchical approach to link the micro-structural characteristics of steel and ductile crack growth resistance curve of a component is proposed. First attention is paid to reveal mechanical properties that control ductile crack growth resistance curve (CTOD-R curve), so that the R-curve could be numerically predicted only from those properties. It is shown from the observation of a mechanism for ductile crack growth that two types of "ductile properties" of steel associated with ductile damage can mainly influence CTOD-R curve; one is a resistance of ductile crack initiation estimated with critical local strain for ductile cracking from the surface of notch root, and the other one is a stress triaxiality dependent ductility obtained with circumferentially notched round-bar specimens. The damage model for numerically simulating the R-curve is proposed taking these two "ductile properties" into account, where ductile crack initiation from crack-tip is in accordance with local strain criterion, and subsequent crack growth triaxiality dependent damage criterion. This macroscopic simulation can correlate the mechanical properties of steel with CTOD-R curve of a component. The second approach is to develop a simulation method to predict the effect of micro-structural characteristics of two-phase steel on the two types of ductile properties that were found to be ductile crack growth controlling mechanical properties. To simulate meso-scale ductile damage behaviors, 3D micro-structural FE-model is developed for analyzing the stress/strain localization behaviors by micro-structural strength mismatch and ductile damage model for reproducing damage evolution up to micro-void/micro-crack formation. This meso-scopic simulation can correlate micro-structural characteristics with mechanical properties of two-phase steel. Through the proposed hierarchical approaches, micro-structural morphology of two-phase steel to improve ductile crack growth resistance of a component can be discussed.

Keywords Damage model, 3D-simulation, Microstructure, Ductile crack growth resistance

1. Introduction

It is necessary to estimate ductile crack growth property of a steel structure for rational assessment of unstable fracture associated with ductile crack initiation and subsequent crack growth. Furthermore, from steel developing side, it should be required to provide a guideline for improving ductile crack growth resistance from *material properties* point of view. On the other hand, it is expected to improve resistance of ductile crack initiation and extension by controlling heterogeneous micro-structure of steel. However, no effective guideline in terms of material properties for improving resistance of ductile crack growth resistance of a cracked structural component has been necessarily established.

For this purpose, the target was focused on proposing a hierarchical approach to link the micro-structural characteristics of multi-phase steel and ductile crack growth resistance of a structural component, which consists of macroscopic approach and mesoscopic approach. Figure 1 describes this concept. The final goal of this study is to develop a numerical simulation method for estimating the effect of micro-structural characteristics of multi-phase steel on ductile crack growth resistance of a structural component.

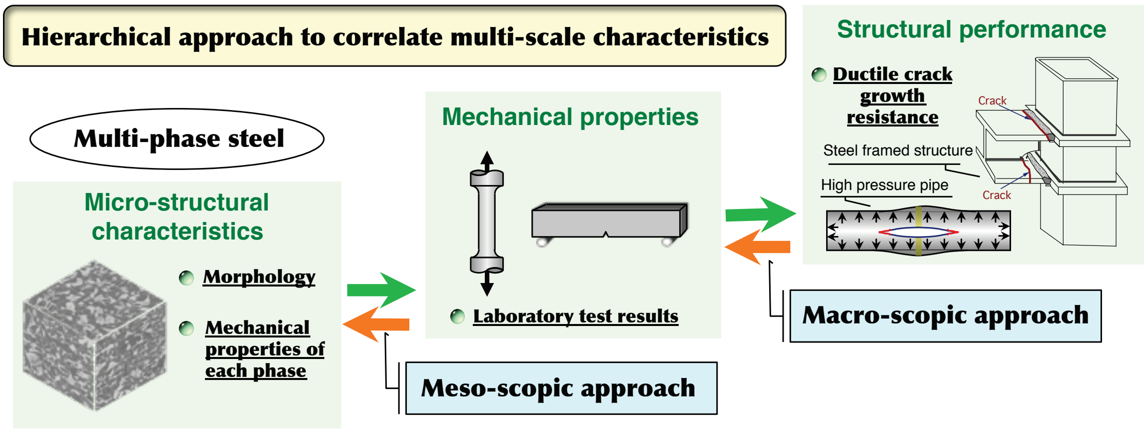


Figure 1. Concept for developing simulation method.

2. Simulation method for correlating ductile crack growth resistance with mechanical properties (Macroscopic approach)

First attention in this study, that is macroscopic approach, was paid to developing a simulation method for correlating ductile crack initiation and extension properties (CTOD-R curve) with mechanical properties that could be obtained by laboratory tests. One of the authors has already proposed the numerical simulation model [1]. The ductile crack initiation from crack-tip is in accordance with *local strain criterion* [1-4], and the subsequent crack extension *triaxiality dependent damage criterion* [1]. This model can predict a CTOD-R-curve only from two types of ductile properties and stress-strain curve of steel; one is a resistance of ductile crack initiation estimated with *critical local strain* for ductile cracking from the surface of notch root obtained with notched bend specimen, and the other one is a *stress triaxiality dependent ductility* obtained with circumferentially notched round-bar specimens. In this chapter, the applicability of this model to prediction of CTOD-R curve of a cracked component of high strength steel is demonstrated.

2.1. Mechanical properties controlling ductile crack growth resistance

The steels used in this study are steels A, B and C. The steels A and B have almost the same yield stress and work hardening, whereas the steel C has higher strength and lower work hardening as shown in Figure 1. Table 1 summarizes the strength properties of all the steels used.

Two types of the ductile properties, which are critical local strain and stress triaxiality dependent ductility, of all the steels that would control ductile crack growth resistance of cracked components were measured.

To measure a critical local strain $(\bar{\varepsilon}_p^{tip})_{cr}$, static 3-point bending tests were conducted using V-notched Charpy specimen. Typical shear mode ductile cracking was observed, which implies that the local strain criterion can be applicable to the steels used. By means of FE-analysis, a critical equivalent plastic strain $(\bar{\varepsilon}_p^{tip})_{cr}$ at crack-tip element was estimated. Another ductile property of the steels, that is stress triaxiality dependent critical local strain $(\bar{\varepsilon}_p)_{cr}$, was examined by conducting tensile test as well as FE-analysis for round-bar specimens with circumferential notch. $(\bar{\varepsilon}_p)_{cr}$ as a function of stress triaxiality were estimated on the middle of the notch-root section where ductile cracking occurred in experiments. The details of the method of experiments and FE-analysis are described in the literature [1]. Figure 2 summarizes the obtained two types of the *ductile properties*. The $(\bar{\varepsilon}_p^{tip})_{cr}$ and tress triaxiality dependent critical local strain $(\bar{\varepsilon}_p)_{cr}$ for the steel C are lower than those for steels A and B. From these results, ductile crack growth resistance for the steel C can be supposed to be the lowest.

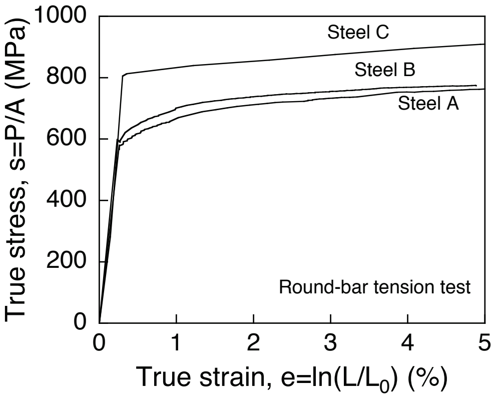


Figure 2. True stress-true strain curves for steels used.

Table 1. Mechanical properties of steels used.

	$\sigma_{0.2}$ (MPa)	σ_T (MPa)	YR	ε_T (%)
Steel A	620	721	0.86	8.5
Steel B	650	735	0.88	5.1
Steel C	829	879	0.94	5.8

$\sigma_{0.2}$: 0.2%proof stress, σ_T : Tensile strength,
ε_T : Uniform elongation (G.L.=32mm),
YR : Yield to tensile ratio ($=\sigma_{0.2}/\sigma_T$)

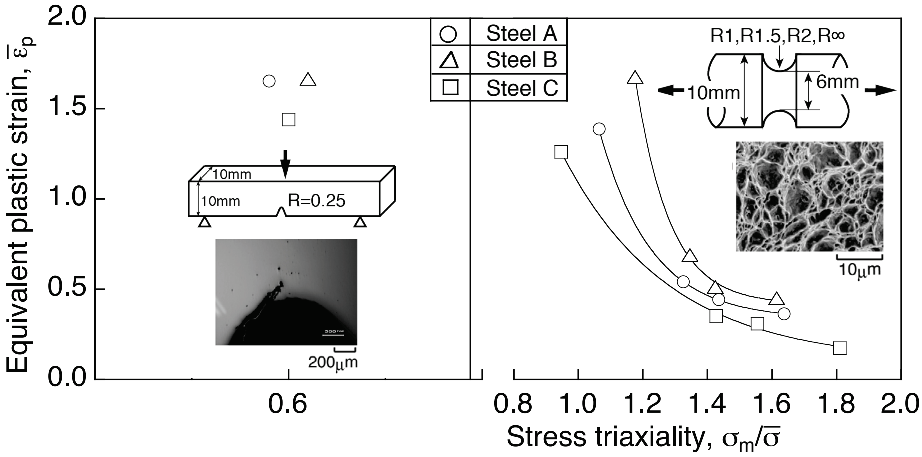


Figure 3. Ductile properties controlling ductile crack growth resistance for steels A, B and C.

2.2. Simulation based prediction of ductile crack growth resistance

2.2.1. Simulation model for ductile crack growth behavior [1]

The damage model for numerically simulating a ductile crack growth resistance, that is R-curve, has been proposed taking the two *ductile properties* of steel into account, where the ductile crack initiation from crack-tip is in accordance with *local strain criterion*, and the subsequent crack growth *triaxiality dependent damage criterion*. The details of the criteria are described in the literature [1]

The *local strain criterion* is applied only for predicting ductile crack initiation from tip of a crack-like defect. In the FE-model, a first element ahead of crack-tip losses a stiffness when an equivalent plastic strain at this element $\bar{\varepsilon}_p^{tip}$ attains to a critical local strain $(\bar{\varepsilon}_p^{tip})_{cr}$ of steel of interest.

The *triaxiality dependent damage criterion* is applied for simulating subsequent ductile crack extension. The proposed yield function, that is the plastic potential, as a function of the damage variable D^* is expressed in Eq. (1),

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

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 a matrix material. This yield function, which is based on a void growth model that was originally proposed by Gurson [6], was derived so that the relation between the critical strain $(\bar{E}_\mathrm{p})_\mathrm{i}$ for micro-voids formation and the stress triaxiality can be in accordance with an exponential function as expressed in Eq. (2).

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

Therefore, the material parameters a_1 and a_2 can be identified only from the stress triaxiality dependent ductility of steel. The $(\bar{E}_\mathrm{p})_\mathrm{i}$ is generally set to be 80% of ductile cracking strain $(\bar{\varepsilon}_\mathrm{p})_\mathrm{cr}$ for the steel which exhibits mico-voids nucleation controlled ductile failure behavior.

2.2.2. Simulation of ductile crack growth resistance of a cracked component.

In the light of two types of ductility of each steel presented in Fig. 3, critical local strain $(\bar{\varepsilon}_\mathrm{p}^\mathrm{tip})_\mathrm{cr}$ and damage parameters a_1 and a_2 were identified. Table 2 summarizes these parameters for all the steels used: D_0, D_c and K are fixed as 0.0001, 0.001 and 4, respectively.

Table 2. Materials parameters used for simulation.

	Initiation	Extension				
	Critical local strain	Damage process based variables			Ductility based variables	
		D_0	D_c	K	a_1	a_2
Steel A	1.6	0.0001	0.001	4	1.54	1.28
Steel B	1.6				0.66	1.59
Steel C	1.4				0.72	1.78

Figure 4 exhibits a FE-model of 3-point bend specimen with a deep crack (a_0/W=0.5) used for simulation, which has the same configuration and size as used in experiments. The simulated ductile crack growth resistance curves, that are CTOD-R curve, were compared with experimental results. As shown in Fig. 5, it was demonstrated that the proposed simulation method could predict CTOD-R curve of the cracked 3PB specimen with high accuracy even for the high strength steel C.

Consequently, by means of the proposed simulation method, a ductile crack growth resistance of a cracked component can be quantitatively correlated with the mechanical properties obtained by laboratory tests.

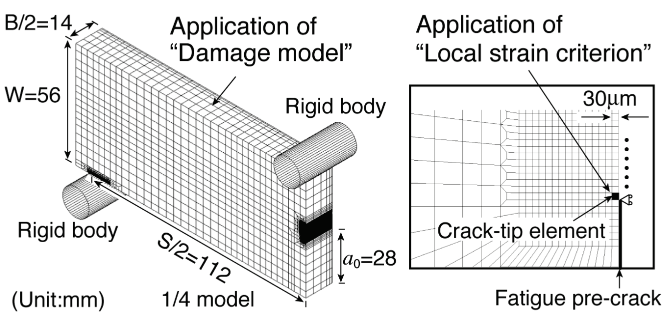


Figure 4. FE-mesh division and simulation model.

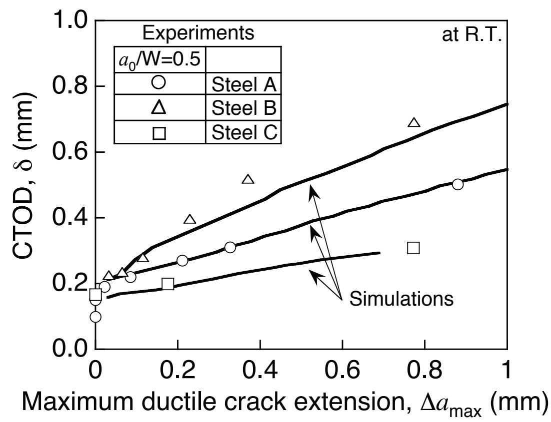


Figure 5. Comparison between CTOD-R curves obtained by experiment and simulation for steels A, B and C.

3. Simulation method for correlating micro-structural characteristics with mechanical properties of two-phase steel (Mesoscopic approach)

Second effort is to develop the mesoscopic method for correlating micro-structural characteristics with mechanical properties of two-phase steel, for instances Ferrite-Pearlite, Ferrite-Bainite, Ferrite-Martensite steel and so on. The authors have proposed a simulation method for predicting the effect of micro-structural morphology on ductile cracking for two-phase structural steel on the basis of micro-mechanism for ductile cracking through the following developments [3-5]: one is a meso-scale 3D micro-structural 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 a damage evolution and subsequent micro-void nucleation model. This model is expected to be able to predict the two ductile properties, which was found in the macroscopic approach to be the mechanical properties controlling CTOD-R curve, as well as stress-strain curves. In this chapter, it is demonstrated that the proposed model could simulate ductile cracking behaviors associated with heterogeneous micro-structure of two-phase, Ferrite-Pearlite, steel. Then, the effect of morphology of micro-structure of two-phase steel on two ductile properties, which are the *critical local strain* and the *stress triaxiality dependent ductility*, is analyzed.

3.1. Ductile cracking behaviors of two-phase steel with heterogeneous micro-structure

The structural steel JIS SM490YB with Ferrite-Pearlite two phases (F-P steel) was used. The hardness of Pearlite phase is about 1.4 times larger than Ferrite phase. Volume fraction of Pearlite phase is about 30 %, the average grain size is about 25 μm.

Table 2. Mechanical properties of SM490YB steel used.

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

σ_Y : Lower yield stress, σ_T : Tensile strength, YR : Yield to tensile ratio $=\sigma_Y/\sigma_T$, ε_T : Uniform elongation
El. : Elongation(G.L. = 36 mm, Dia. = 6 mm), Hv : Average Vickers hardness (Load : 25 gf)

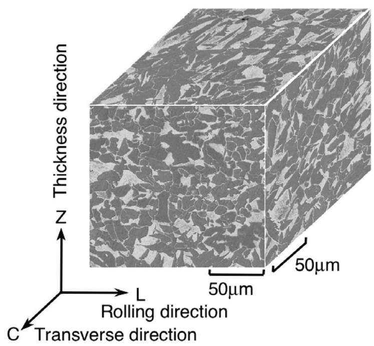


Figure 6. Microstructures of SM490YB steel used.

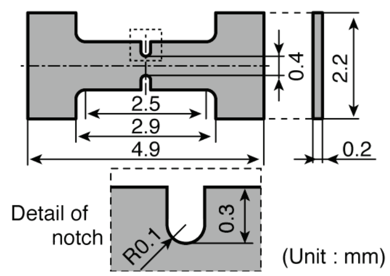


Figure 7. Configuration of notched micro-tensile specimen used.

The specimen for observing ductile cracking behaviors is flat micro-tensile specimen with side notches, as shown in Fig. 7. Figure 8 presents load P and displacement u curves obtained by tensile testing for three specimens. The specimens were unloaded at levels 1 and 2, and observed damage evolution up to failure. The ductile cracks generated from not only notch-root surface but also middle of net section, that is inside of the specimen, were observed at loading level 2, as shown in Fig. 9. These micro-cracks seem to mainly nucleate at Ferrite side with lower hardness near Ferrite-Pearlite boundary. This implied ductile damage was localized by stress/strain concentration that would be due to micro-structural strength mimatch. The other important point to be notice is that no large voids associated with non-metallic inclusions were found after large amount of plastic straining, as is observed in the cross section at loading level 1.

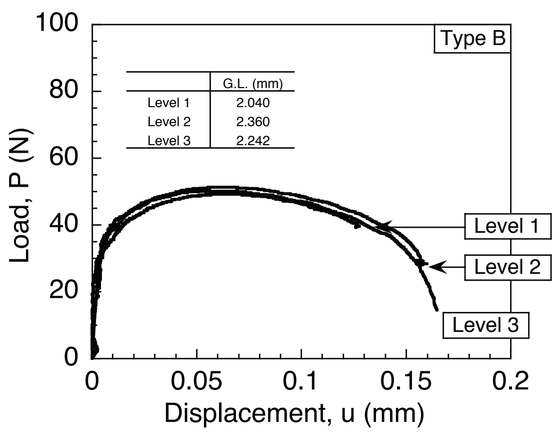
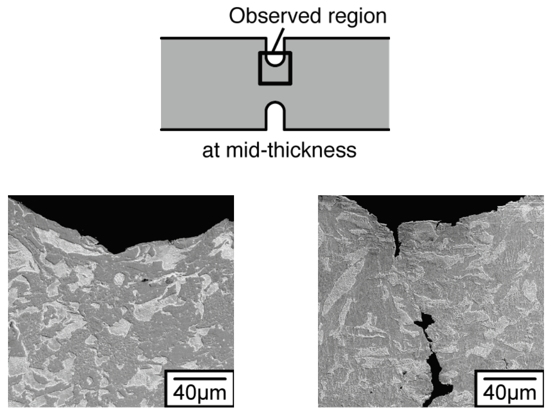


Figure 8. Load - displacement curves obtained by tensile tests for micro-tensile specimen with side notches.



(a) Level 1 (b) Level 2

Figure 9. Ductile damage evolution in notched micro-tensile specimen.

3.2. Simulation method of ductile cracking behavior associated with heterogeneous micro-structure

In order to simulate ductile cracking behaviors associated with heterogeneous micro-structure of two-phase steel, ductile damage simulation method was proposed [5]. Figure 10 shows the conceptual illustration of this method. According to this method, ductile cracking behaviors of two-phase steel can be predicted from the following characteristics of constituent phase by using 3D micro-structural model; one is two kinds of mechanical properties i.e., strength property and damage property. The former is stress-strain curve, and the later is stress triaxiality dependent ductility. Another one is morphology of micro-structure of steel, for instances size and aspect ratio of grain size, volume fraction of second phase, connectivity of matrix phase and so on. In this method, the same numerical damage model as that used in the macroscopic approach is applied.

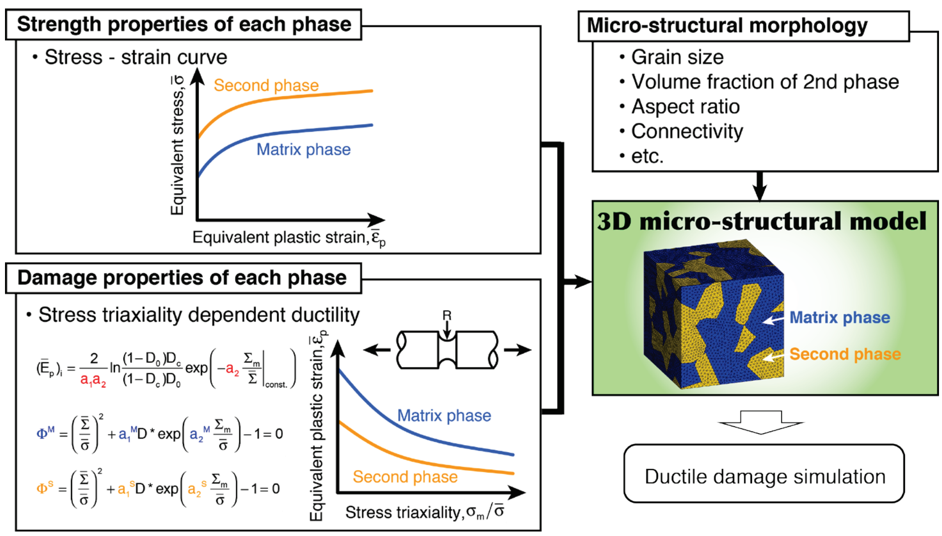


Figure 10. Conceptual illustration of the mesoscopic simulation method.

A simulation model of the micro-tensile specimen that has the same configuration of that used in the experiment is shown in Fig. 11. 3D micro-structural model is employed only around the net section. 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, and element size 5μm.

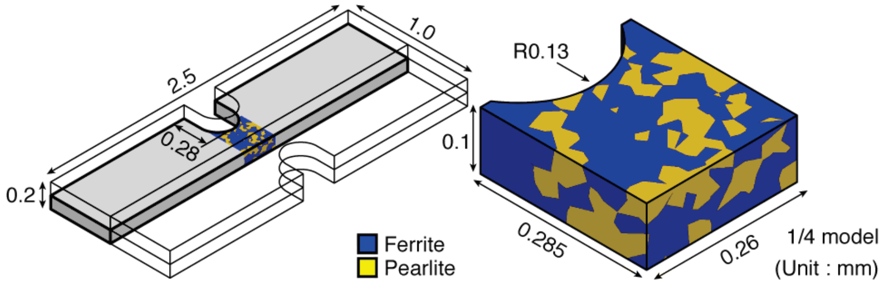
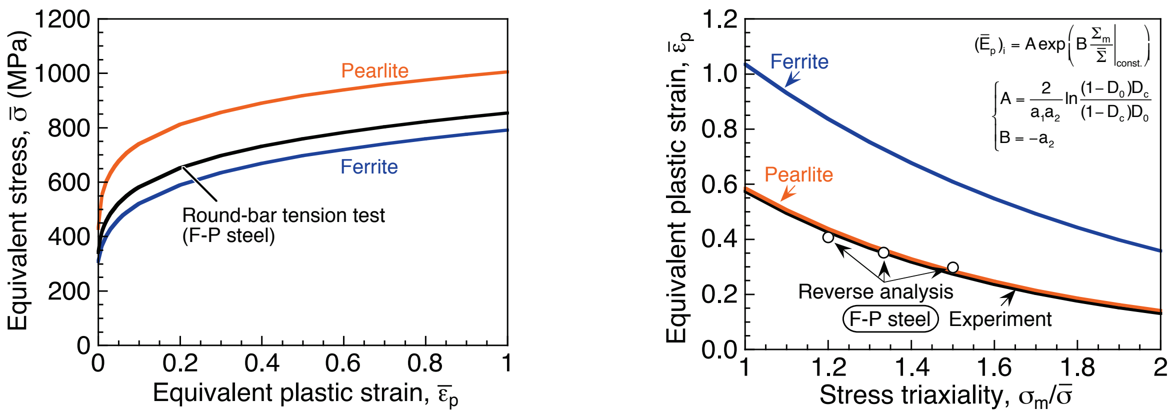


Figure 11. Meso-scale 3D FE-model of flat micro-tensile specimen with side notches.

The mechanical properties needed for the proposed simulation can be identified from testing for full Ferrite and full Pearlite steels having the same morphological and metallurgical properties as those of each phase in F-P steel used. However, in this work, some assumptions were employed for identifying those properties. As for the stress-strain curves of Ferrite and Pearlite phases, they were estimated in accordance with a rule of mixture from stress-strain curve of two-phase steel used [5]. Figure 12(a) shows the equivalent stress $\bar{\sigma}$ – equivalent plastic strain $\bar{\varepsilon}_p$ curves for the Ferrite and Pearlite phase along with that obtained by tension test for F-P steel used. The damage parameters for the each phase can be obtained by conducting tension tests for round-bar specimens with/without circumferential notches in accordance with the proposed procedure (section 2.2). However, these parameters were determined based on the stress triaxiality dependent ductility for the F-P steel as presented in Fig. 12(b). The properties for the Ferrite phase were identified by reverse analysis so that the stress triaxiality dependent ductility for the F-P steel might be reproduced by simulation using a 3D micro-structural model (see Fig. 15(b)). As for the Pearlite phase, the same properties as those for F-P steel were used, because no significant effect of those parameters on simulated result was found in this case.



(a) Stress-strain curve (b) Stress triaxiality dependent ductility

Figure 12. Mechanical properties of constituent phases of F-P steel needed for damage simulation.

Figure 13 shows *P*–*u* curves obtained by experiment and simulation. The simulation reproduces critical tensile displacement where load drop due to ductile cracking occurred. Ductile damage evolution behaviors from notch root surface and middle of the specimen obtained by simulation are well consistent with experimental results, and damage localization in Ferrite phase near Ferrite/Pearlite boundary is well simulated as shown in Fig. 14.

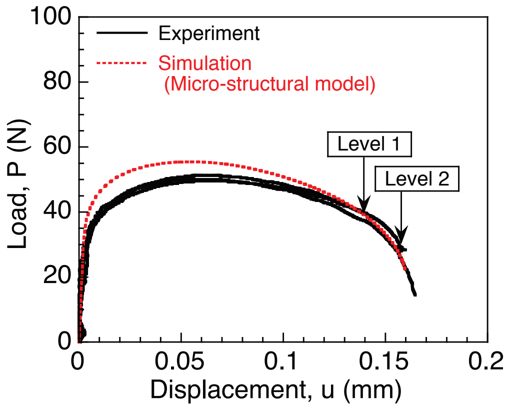


Figure 13. Load - displacement curves obtained by experiment and simulation for notched micro-tensile specimen.

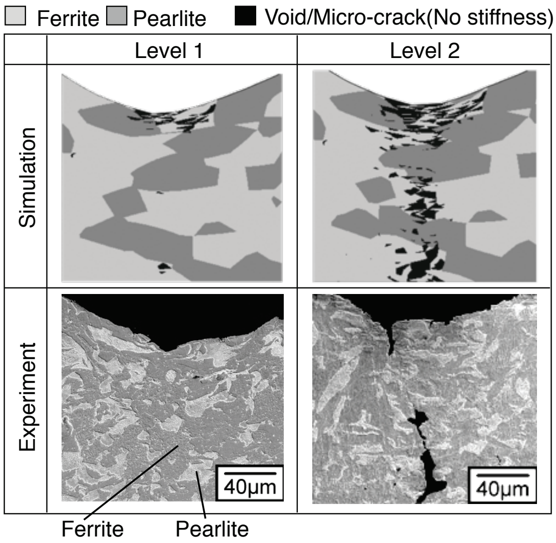
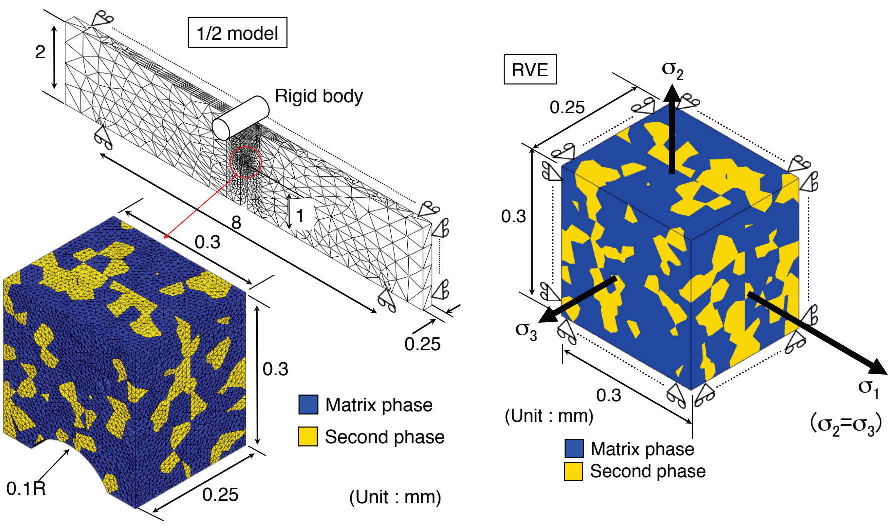


Figure 14. Comparison between simulated and observed ductile damage evolution for notched micro-tensile specimen.

3.3 Effect of micro-structural morphology on mechanical properties

It is demonstrated that the developed simulation model can well simulate ductile cracking behaviors regardless of surface or inside of a specimen, namely regardless of global triaxial stress conditions. Therefore, effect of micro-structural characteristics of two-phase steel on the macro-scopic ductile properties i.e., critical local strain and stress triaxiality dependent ductility which were found to control ductile crack growth resistance of a cracked component could be expected to be able to predict on the basis of the meso-scopic simulation method.

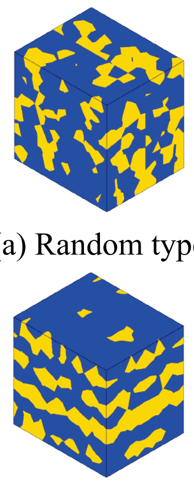
Simulation model to estimate those macro-scopic ductility are proposed as given in Figure 15; (a) is 3-point bend specimen with sharp crack for critical local strain and (b) is tensile RVE (Representative Volume Element) under constant stress triaxiality for stress triaxiality dependent ductility, which controls macro-scopic ductile crack initiation and extension, respectively.



(a) For critical local strain

(b) For stress triaxiality dependent ductility

Figure 15. Models for simulating the effect of micro-structural characteristics of two-phase steel on ductility.



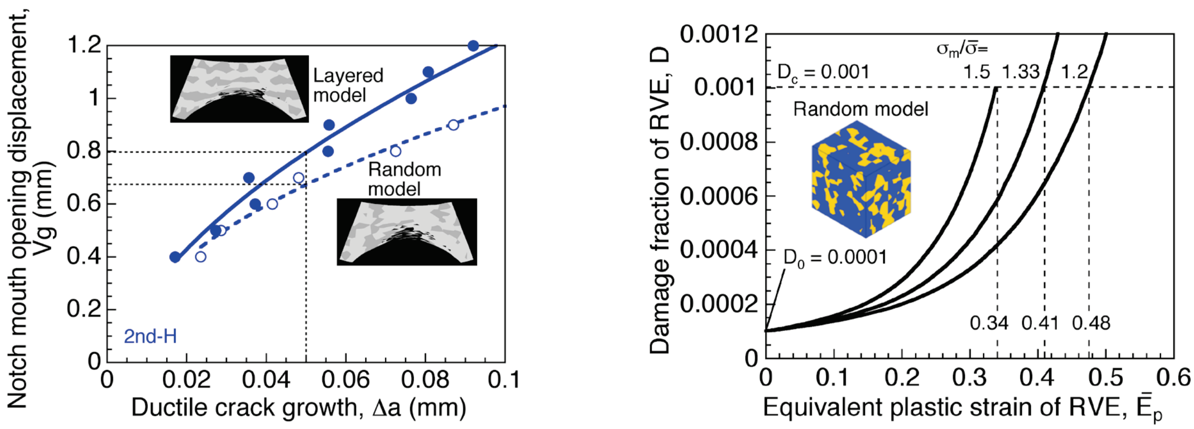
(a) Random type

(b) Layered type

Figure 16. Type of morphology of micro-structure

As a case study, effect of second phase (harder phase) distribution of two-phase steel is estimated using a random type and layered type morphology as presented in Fig. 16. Both types have the same volume fraction of the second phase of 30%, and the same average grain size of 25μm. The matrix and second phases are assumed to be Ferrite and Pearlite, respectively, and the mechanical properties given in Fig. 12 are used for damage simulation.

Results of simulated damage evolution are presented in Fig. 17. Critical global deformation for ductile cracking from notch root surface, which is defined as Vg where ductile crack growth Δa reaches 50μm, can be obtained from the 3-point bending simulation (Fig. 17(a)). Then, in contrast to the FE-analytical results for homogeneous material model of the 3PB specimen, macro-scopic critical local strain $(\bar{\varepsilon}_p^{tip})_{cr}$ can be estimated. Figure 17(b) gives evolution of damage fraction D of RVE as a function of macro-scopic equivalent plastic strain $\bar{E}_p$. The stress triaxiality dependent ductility that is defined as $\bar{E}_p$ where D reaches 0.001 (=D_c) can be estimated.



(a) For critical local strain (b) For stress triaxiality dependent ductility

Figure 17. Damage simulation to estimate the effect of micro-structural morphology of two-phase steel on macro-scopic ductility.

Figure 18 summarizes the estimated macro-scopic critical local strain $(\bar{\varepsilon}_p^{tip})_{cr}$ and stress triaxiality dependent ductility for the random and layered type morphology of F-P steel. It was predicted that the layered type morphology provided larger macro-scopic ductility than the random type morphology as long as a volume fraction of second phase were the same. Therefore, the layered type morphology could enlarge ductile crack growth resistance of a cracked structural component.

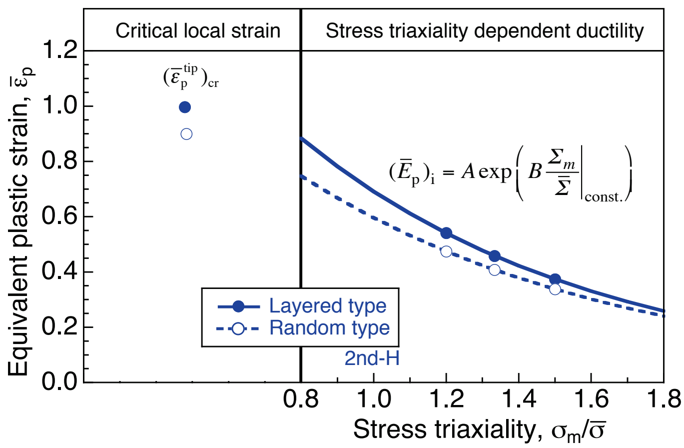


Figure 18. Effect of micro-structural morphology of two-phase steel on macro-scopic ductility simulated on the basis of the proposed meso-scopic approach.

4. Conclusions

In this work, hierarchical approach to link the micro-structural characteristics of multi-phase steel and ductile crack growth resistance of a structural component was proposed (see. Fig. 19). This approach consists of *macro-scopic approach* and *meso-scopic approach*. The macro-scopic approach can provide a guideline to control mechanical properties for improving ductile crack growth resistance of a cracked structural component. And the meso-scopic approach can correlate micro-structural characteristics with mechanical properties of two-phase steel. Through the proposed hierarchical approach, micro-structural characteristics of two-phase steel to improve ductile crack growth resistance of a structural component can be discussed, however further verification works should be conducted.

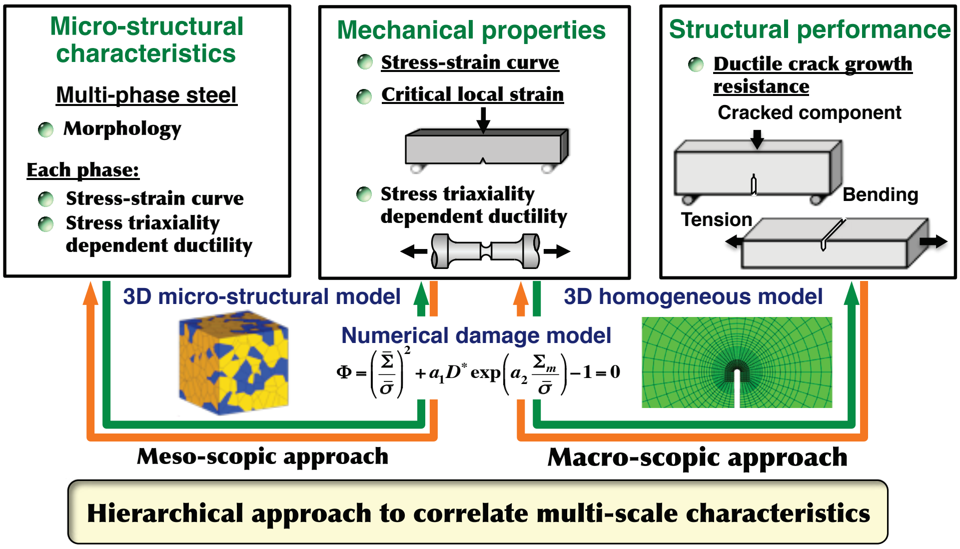


Figure 19. Hierarchical approach to correlate multi-scale characteristics i.e., micro-structural characteristics, mechanical properties and structural performance.

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