Multiscale modeling to clarify the relationship between microstructures of steel and macroscopic brittle crack propagation/arrest behavior

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Abstract

Prevention of brittle crack propagation as well as crack initiation is essential as “double integrity”. The application of steels with high arrestability to the structures is directly effective to ensure the integrity. Although it is empirically known microstructures have a possibility to macroscopically enhance the arrestability of steel, there are not any theories which have quantitatively explained the relationship between brittle fracture and microstructures in the past investigations. In the present study, we propose a multiscale fracture mechanics model by a “model synthesis” approach, which integrates the multiple models and analyses to systematically evaluate complicated macroscopic and microscopic phenomena, based on the information of microstructures of the steel. The model is composed of (i) microscopic model to simulate cleavage fracture in grain scale (10−6~10−3 m), and (ii) macroscopic model to simulate brittle fracture in steel plate scale (10−3~100 m). As validation, the proposed model is applied to temperature gradient crack arrest test of steel plate having nonhomogeneous distributions of microstructures in thickness direction. The prediction results show good agreement with experimental results in both crack arrest length and shape of crack front. That is, the proposed model has a potential basis of the framework to establish the theory to clarify the relationship between microstructures and brittle crack propagation and arrest behavior.

Keywords: brittle fracture; multiscale model; model synthesis; Monte Carlo simulation; cleavage fracture; crack propagation; crack arrest

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1. Introduction

Recently, increasing strength and thickness of steel plate are promoted due to the requirement of the significant enlargement for many ships and offshore plants in the heavy industries. It is considered that the increase of the thickness in steel makes the risk of brittle fracture higher. In addition, for such large steel structures, weld joints are frequently used, which can cause deterioration in toughness. It is actually difficult to remove welding defects fatigue cracks by repeated load during service completely. As a “double integrity”, prevention of brittle crack propagation as well as crack initiation is thus essential for large steel structures.

The application of steels with high arrestability to the structures is directly effective to ensure the integrity. Therefore, there have been a lot of efforts on researches and developments of the steels with higher arrestability. In particular, it has been recognized that there is a strong correlation between microstructures and arrest toughness as an empirical knowledge supported by many experiment such as Ohmori et al. (1976) and Shirahata et al. (2014).

As mentioned above, in the recent years, the high strength steels have been widely spread for actual use. They are generally made by low temperature rolling, so that the high strength steel shows not only stronger texture but also more nonhomogeneous distributions of grain size and orientation in the thickness direction than the conventional steels. It was reported that such a state of microstructures has a possibility to macroscopically enhance the arrestability of steel by Handa et al. (2012). In particular, a steel plate with higher arrestability at the mid-thickness position rather than at the quarter-thickness position shows a characteristic and complicated fracture surface morphology, called as “split-nail”, and also shows higher brittle crack arrest performance, which was reported by Tsuyama et al. (2012). However, there are not any theories which have quantitatively explained the relationship between brittle fracture and microstructures in the past investigations.

According to the above mentioned facts, in the present paper, we propose a multiscale model to simulate the complex behavior of brittle crack propagation and arrest based on the information of microstructures of the steel in order to clarify the relationship between brittle crack propagation/arrest behavior and microstructures.

2. Concept of the multiscale model

One of the most major problems to be solved is a large “scale gap” between macroscopic and microscopic phenomena. Brittle fracture of the steel plate is generally in the scale of $10^9$m. On the other hand, the microstructures as polycrystalline are generally in the scale of $10^{-8}$$~10^{-4}$m, and moreover, the cleavage fracture condition on a crystal is in the scale of $10^{-9}$m. In addition, the brittle fracture in steel occurs in the significantly fast process with extremely strong material nonlinearity, which is difficult to be experimentally measured in detail.

In the present paper, we show the first attempt to solve the problem of the scale gap between macroscopic and microscopic phenomena by a new proposal of multiscale model by a “model synthesis” approach. Fig.1 shows an outline of the proposed multiscale model, whose detail contents are found in Shibanuma et al. (2016) and Yamamoto et al. (2016). The multiscale model consists of two models: (1) a microscopic model and (2) a macroscopic model. The microscopic model simulates cleavage fracture in the grain scale. The macroscopic model simulates brittle fracture in the steel plate scale. The same framework for domain discretization and criterion of crack propagation is used in both the models for simplification.

2.1. Domain discretization and criterion of crack propagation

The framework is developed based on the model of McClintock (1997) and Aihara et al. (2011) which simulates microscopic cleavage fracture.

Brittle crack propagation and arrest behavior in steel is the significantly fast process with extremely strong material nonlinearity. In particular, the crack path shows a complicated three-dimensional morphology. In the present study, the three-dimensional crack propagation is simulated quasi-three-dimensionally as follows: the entire domain is divided into rectangular unit cells, then the crack propagation is modeled by a step-by-step calculation. Fig.2 shows the schematic of the domain discretization and crack propagation modeling.

The entire domain for the microscopic model is defined as a square whose size is 1mm by 1mm in the width and thickness directions of a plate, respectively. The entire domain is divided into square unit cells with the same size
which is equal to mean grain size. That is, each unit cell simulates a grain of steel in the microscopic model. On the other hand, the entire domain for the macroscopic model is defined as an actual plate size. The entire domain is divided into the square unit cells. Each unit cell corresponds to the entire domain of the microscopic model, so that the size of the unit cell in the macroscopic model is 1 mm by 1 mm in the width and thickness directions.

The crack propagation is evaluated by the criterion comparing between driving force and resistance of crack propagation in terms of stress intensity factor, as

\[ k \geq k_f \]  \hspace{1cm} (1)

where \( k \) is the equivalent stress intensity factor as the driving force of crack propagation, and \( k_f \) is the fracture toughness as the resistance of crack propagation.

In the microscopic model, \( k_f (= k_{f_{m}}) \) is defined as a material constant. On the other hand, in the macroscopic model, \( k_f (= k_{f_M}) \) is calculated from the result of the microscopic model. Calculation of the stress intensity factor \( k \) in Eq.(1) is performed by a superposition of the approximate solutions for the effect of three crack shapes: (1) non-straightness of the crack front, (2) non-planar of the crack surface, and (3) crack closure effect by the tear-ridge. In this calculation, the approximated effects of various crack shapes are superposed on the stress intensity factor for a crack having flat surface and straight crack front perpendicular to the crack propagation direction in the infinite body, \( k_{1}^{\infty} \), as

\[ k_{1}^{\infty} = \sigma_{yy}[r_c]\sqrt{2\pi r_c} \]  \hspace{1cm} (2)

where \( r_c \) is the characteristic length, assumed as \( r_c = 0.2 \text{mm} \), \( \sigma_{yy} \) is tensile stress in front of the crack tip, which is obtained by the dynamic elasto-plastic finite element analysis performed in the macroscopic model.

Fig.3 shows the schematic of the criteria and approximate calculation of the stress intensity factor.

2.2. Microscopic model

The calculation by the microscopic model is performed for simulating the cleavage fracture with the input data of grain size and orientation. The aim of the calculation is evaluation of (1) effective surface energy, and (2) direction of fracture surface. These quantities used as input data in the macroscopic model.

Brittle fracture in steel is microscopically the continuation of cleavage fracture in grains. Cleavage fracture surfaces are known to form on \{100\} planes in a BCC polycrystal including ferrite as reported in Shibanuma et al. (2012).
Considering the above, the entire domain whose size is 1mm by 1mm, which corresponds to a unit cell in the macroscopic model, is discretized into square unit cells of the average grain size $\bar{d}$, so that each unit cell corresponds to a grain of steel. The stress tensor is assumed to act on the entire domain constantly because the entire domain is sufficiently small. The grain orientation is assigned to each unit cell to define \{100\} planes of the grain according to the distribution of the grain orientation. Fracture surfaces at each unit cell is simulated by selecting the \{100\} plane which the maximum normal stress is acting on as the following expression.

$$\sigma_{n}^{max} = \max_{m=1,2,3} (n_{m})^T \cdot \sigma[r, \theta_{m}] \cdot n_{m} \quad (3)$$

where $n_{m}$ is a unit normal vector of the $m$-th \{100\} plane and $\sigma$ is stress tensor near crack tip as the following expression.

$$\sigma[r, \theta] = \frac{1}{\sqrt{2\pi}t} \sum_{i=1}^{3} k_{i} f_{i}[\theta] \quad (4)$$

where $f_{i}[\theta]$ is coefficient tensor functions of $\theta$ corresponding to the fracture mode $i$. Crack propagation and arrest behavior are simulated by successively evaluating the criterion expressed by Eq.(1) at crack tip unit cell.

For the integration of the microscopic model into the macroscopic model, two physical quantities are used: (1) effective surface energy $\gamma$, and (2) direction of fracture surface $n_{M}$. As mentioned above, the entire domain in the microscopic model corresponds to the unit cell in the macroscopic model, so that these quantities can be calculated from the fracture surface obtained by the microscopic model.

The energy absorbing mechanism during brittle crack propagation has not been sufficiently clarified. In the present study, we assume that the plastic work to form tear-ridge is dominant in the total absolute energy to form the macroscopic fracture surface. The energy to form the tear-ridge can be calculated by the following formula.

$$\gamma = \frac{1}{2A} \int_{S} \tau_{\gamma} Y_{cm} ds \quad (5)$$

where $A$ is an area of the entire domain, $\tau_{\gamma}$ is shear strength, $c$ is a ratio of width and height of uncracked ligament, $s$ is grain boundaries, $Y_{cm}$ is critical shear strain. In the present study, two constants, $c$ and $Y_{cm}$, were assumed as $c = 0.1$ and $Y_{cm} = 0.7$ in reference to the past study by Sugimoto et al. (2014). Fig.4 shows an optical microscope photograph of tear-ridge and energy absorption by ductile fracture of tear-ridge. For the calculation of Eq.(1) in the macroscopic model, the arrest toughness $k_{FM}$ is calculated based on the linear elastic fracture mechanics theory, as

$$k_{FM} = \sqrt{2E\gamma} \quad (6)$$

where $E$ is a Young’s modulus.

The direction of fracture surface $n_{M}$ is obtained as the normal vector of approximated plane of the cleavage fracture surface by the least square method.
2.3. Integrated macroscopic model

The integrated macroscopic model is formed as the multiscale model by a new approach of “model synthesis” by systematically incorporating (1) the preparatory macroscopic finite element analysis and (2) the Monte Carlo simulation for the microscopic analysis into (3) the macroscopic analysis for crack propagation and arrest. That is, the integrated macroscopic model is composed of the three-staged analyses. Fig. 5 shows the procedures of the respective analyses in the integrated macroscopic model. The integration procedure is implemented by a one-way coupling algorithm for simplification.

- (a) Preparatory macroscopic finite element analysis
  The aim of the preparatory macroscopic finite element analysis is to obtain (1) stress tensor $\sigma$ and (2) yield stress $\sigma_y$ at the characteristic distance, which is assumed as $r_c = 0.2 \text{mm}$. $\sigma$ and $\sigma_y$ is mainly used for the calculations of the local stress intensity factor $k$ in the following (b) Monte Carlo simulation of microscopic analysis for cleavage fracture and (c) integrated macroscopic analysis by model synthesis.

The analysis was performed under the dynamic elastic-plastic condition without considering non-linearity of geometry. We employed the regression formula by Goto et al. (1994) as the yielding condition. The true stress-strain curve is approximated by the Swift’s equation. The strain hardening exponent is assumed to satisfy the regression formula by Toyosada et al. (1992).

The nodal force release method is employed to simulate fast crack propagation. For simplification, the crack surface is assumed to be flat vertically to the loading direction and the shape of crack front is straight perpendicular to the crack propagation direction. Crack velocity is fixed as $V = 500 \text{m/s}$ assumed to be just before crack arrest. The entire size of the model is decided by comparing the elastic Rayleigh wave velocity with the crack velocity so that the reflection of elastic wave at the boundaries did not interfere with the crack. The minimum element size along a crack is 0.05 mm, which is determined to be smaller than the characteristic length of $r_c = 0.2 \text{mm}$ for the assurance of accuracy. Fig. 6 shows an example of the mesh and entire model of the finite element analysis.

- (b) Monte Carlo simulation of microscopic analysis for cleavage fracture
  The Monte Carlo simulation for microscopic model analysis as the second stage of the integrated macroscopic model is performed at the discrete evaluation points of the plate for efficiency of the whole analysis. A schematic of the microscopic analysis is shown in Fig. 7. The input data of the microscopic model are (1) average grain size $\bar{d}$, (2) distribution of grain orientation, (3) remote applied stress tensor $\sigma$ and (4) yield stress $\sigma_y$, at each evaluation point. Sufficient number of trials of the Monte Carlo simulation is required to make reasonable distributions of (1) the fracture toughness $k_{FM}$ and (2) the direction of fracture surface $n_M$.

- (c) Macroscopic analysis by model synthesis
  The integrated macroscopic model as the multiscale model bridging the large gap in scale is simulate the macroscopic brittle fracture on the plate scale.
The procedure in the integrated macroscopic model is composed of the two parts, i.e., in the part 1: assignment of the results ($\sigma$ and $\sigma_y$) obtained by the above (1) the preparatory macroscopic finite element analysis and ($k_{TM}$ and $n_M$) obtained by the above (2) the Monte Carlo simulation of the microscopic analysis in each unit cell, and in the part 2: simulation of crack propagation and arrest by the above (3) the macroscopic analysis.

### 3. Application to crack arrest test for model validation

For the model validation we proposed in the present study, the model is applied to the temperature gradient crack arrest test of the steel plates having nonhomogeneous distributions of microstructures in thickness direction.

#### 3.1. Test steel and Experiment

Table. 1 shows chemical compositions of the test steel.

The steel plate was rolled to 60mm in thickness under controlled temperature condition, hence it has nonhomogeneous distributions of microstructures in thickness direction. Table 2. shows (1) optical microscope photographs, (2) EBSD maps, (3) averaged grain sizes, (4) {100} pole figures, and (5) strengths of texture, for surface, in the quarter-thickness and mid-thickness of the plate, respectively. The width of the test plate is 300mm and yield stress is 394MPa.

The experiment for temperature gradient crack arrest test was conducted in accordance with the standard, WES 2815, by The Japan Welding Engineering Society (JWES) (2014). Fig. 8. shows schematic of the temperature gradient crack arrest test. Applied stress was set as $\sigma_{app} = 177$MPa. Temperature gradient near the arrested point was approximately $dT/dx = 0.55 °C/mm$ in the width direction, where $x$ is a coordinate in the width direction. A brittle crack was initiated by air-hammering.

The experiment was conducted under the above conditions. Fig. 9. shows the results of temperature distribution and arrested crack length. Fig. 10 shows fracture surfaces obtained by the crack arrest test. The brittle crack was arrested at 154mm and the crack arrest temperature was $T = −9.2°C$. The fracture surface presents a typical morphology called as “split-nails”, where the crack front at the mid-thickness position retreats from that at the quarter-thickness position as noted in Fig. 10.

#### 3.2. Model simulation and discussion

The proposed multiscale model is applied to the temperature gradient crack arrest test mentioned above, where the brittle crack behavior after the crack length of 60mm was simulated in the present simulation for considering the influence of the impact loading.
The result of fracture surfaces at each crack length is shown in Fig.11. The crack was arrested at 158mm in the simulation. The arrested crack length in the simulation was accurately consistent with that in the experiment of 154mm. Fig.12 shows a comparison between experimental and simulation results of the fracture surface in the xz view and gaps of unit cell boundary. It is found that the proposed model successfully simulated the split nail and chevron pattern.

According to the above discussion, the proposed multiscale model has successfully simulated the complicated brittle crack propagation/arrest behavior for the steel plate having nonhomogeneous distributions of microstructures in the thickness direction. Hence, it is found that the proposed model has been validated from the results of the comparison between the proposed model simulation and experiments.

4. Conclusion

The present paper proposed a new multiscale model by a “model synthesis” approach, as the first attempt to clarify the relationship between microstructures of steel and macroscopic brittle crack propagation and arrest behaviour. The multiscale model is composed of (i) microscopic model to simulate cleavage fracture in grain scale ($10^{-6}$~$10^{-3}$ m), and (ii) macroscopic model to simulate brittle fracture in steel plate scale ($10^{-3}$~$10^{0}$ m).

As validation, the proposed model is applied to temperature gradient crack arrest test of steel plate having nonhomogeneous distributions of microstructures in thickness direction. The multiscale model successfully simulates the experimental results in both crack arrest length and shape of crack front.

The proposed model was developed by the “model synthesis” approach, so that it is able to add and to improve
the components in the model for more detailed discussion in the future. That is, the proposed model in the present study has a potential basis of the framework to establish the theory for the clarification of the relationship between microstructures of steel and macroscopic arrest toughness of steel plate, which was not sufficiently investigated in the past.

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