Multiscale Model Synthesis to Clarify the Relationship between Microstructures of Steel and Macroscopic Brittle Crack Arrest Behavior - Part II: Application to Crack Arrest Test

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The second part of the present paper shows an application of the proposed multiscale model to the temperature gradient crack arrest test of the steel plates having nonhomogeneous distributions of microstructures in thickness direction. The multiscale model is developed as the integrated macroscopic model composed of the three-staged analyses. The first stage is a preparatory macroscopic finite element analysis, where the nodal force release method is employed to simulate fast crack propagation under the dynamic elastic-plastic condition without considering non-linearity of geometry. The second stage is the Monte Carlo simulation of microscopic analysis for cleavage fracture at the discrete evaluation points. The results of local fracture toughness and direction of fracture surface show large scatters even at the same evaluation point. The final stage is the integrated macroscopic analysis, which is composed of the two parts: (a) assignment of parameters obtained in the previous analyses in each unit cell, and (b) simulation of brittle crack propagation/arrest behavior. As a result, the proposed multiscale model successfully simulated the complicated brittle crack propagation/arrest behavior. In particular, not only the arrested crack length but also the characteristic fracture surface such as “split nails” were accurately simulated. It is therefore found that the proposed model has been validated by the comparison with experiment. 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.

KEY WORDS: brittle fracture; multiscale model; model synthesis; Monte Carlo simulation; cleavage fracture; crack propagation; crack arrest; arrest toughness; texture; split nails.

1. Introduction

The controls of crack arrest as well as brittle fracture initiation provide “double integrity” for large steel structures such as ships and offshore structures.¹,²) Therefore, the establishment of the crack arrest concept is essential for the integrity of some large structures whose accidental failure may involve significant social damages.

There have been a lot of works on researches and developments of the steels with higher arrestability, because the application of steels with high arrestability to the structures is directly effective to ensure the integrity of some large structures whose accidental failure may involve significant social damages.

The most major reasons is caused by a large “scale gap” on the dominant factors between macroscopic and microscopic phenomena. The integration between microscopic and macroscopic models to simulate the complex behavior of brittle crack propagation and arrest is required to bridge a large scale gap between 10⁰ m in macroscopic scale and 10⁻³⁻¹⁰⁻⁴ m in microscopic scale.

In the first part of the present paper, we propose a new multiscale model by a “model synthesis” approach, as the first attempt to clarify the relationship between microstructures and macroscopic brittle crack propagation/arrest behavior in steel plate. The multiscale model consists of two models: (1) a microscopic model to simulate cleavage fracture in the grain scale and (2) a macroscopic model to simulate brittle crack propagation and arrest behavior in the steel plate scale. The both models were developed base on the same framework, where a simple two-dimensional domain discretization is employed but a three-dimensional crack propagation can be effectively modeled. The discretized unit cells in the microscopic model correspond to the grain size. On the other hand, the discretized unit cells

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in the macroscopic model correspond to the entire domain of the microscopic model. The microscopic model proposed by Aihara and Tanaka is basically employed except the integration with the macroscopic model. The proposed model synthesis for multiscale model as an integrated macroscopic model is performed by systematically incorporating (1) the preparatory macroscopic finite element analysis and (2) the Monte Carlo simulation of microscopic analysis into (3) the macroscopic analysis for brittle crack propagation and arrest in steel plate. The integration procedure is implemented by the assignment of physical quantities based on the interpolation methods as a one-way coupling algorithm for simplification.

The aim in the second part of the present paper is to validate the new multiscale model proposed in the first part of the present paper by comparing with the experiment of crack arrest test of the steel plates having nonhomogeneous distributions of microstructures in the thickness direction.

2. Temperature Gradient Crack Arrest Test

A temperature gradient crack arrest test is one of the major tests to evaluate crack arrest toughness $K_{ca}$ of a steel plate. The method of the test was published as a standard, WES 2815, by The Japan Welding Engineering Society (JWES). The standard precisely specifies the testing conditions, including specimen configurations, impact energy limit, applied stress limit, etc. based on the related works. The configuration of the temperature gradient crack arrest test is shown in Fig. 1.

$K_{ca}$ is a material parameter compared with stress intensity factor $K$ based on the linear fracture mechanics theory. That is, in the case of $K < K_{ca}$, brittle crack can be arrested. It is known that $K_{ca}$ increases according to the temperature, so that a crack is arrested at the location of $K = K_{ca}$ in the temperature gradient crack arrest test. Thus, $K_{ca}$ can be evaluated as

$$K_{ca} = \sigma_{app} \sqrt{\pi a} \left( \frac{2W}{\pi a} \tan \left( \frac{\pi a}{2W} \right) \right)^{1/2} \quad \text{(1)}$$

where $\sigma_{app}$ is applied stress and $a$ is arrested crack length. Equation (1) is called as the tangent formula, considering the effect of the specimen width $W$.

3. Model Validation

A brittle crack propagation and arrest behavior in a steel plate having nonhomogeneous distributions of microstructures in the thickness direction is simulated for validation of the proposed multiscale model. This section is composed of three parts. Firstly, the test steel for temperature gradient crack arrest test is described in Section 3.1. Second-

| Location | Mid-thickness | Quarter-thickness | Surface |
|----------|---------------|------------------|---------|
| Optical microscope photograph | | | |
| EBSD map | | | |
| Average grain size [μm] | 26 | 22 | 22 |
| $\{100\}$ pole figure | | | |
| Integration degree of $\langle 001 \rangle < 110 \rangle$ direction | 4.1 | 0.7 | 3.1 |
ary, the details of experimental conditions and results for temperature gradient crack arrest test are shown in Section 3.2. Finally, the application of the proposed model and its comparison with the experimental results are shown in Section 3.3.

3.1. Test Steel

Table 1 shows chemical compositions of the test steel. The steel plate was produced by a controlled temperature rolling to 60 mm in thickness so that it has nonhomogeneous distributions of microstructures in the 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 EBSD maps were obtained by OIM analysis software.\(^{16}\) Distributions of equivalent circle diameter and the \{100\} pole figures were extracted from the EBSD map data. The distributions of equivalent circle diameter are shown in Fig. 2. The average grain sizes were calculated as the mean area diameters obtained from the distributions of equivalent circle diameter.

In addition, Table 3 shows the mechanical properties in the rolling direction of the test steel.

3.2. Experiment

In the experiment for temperature gradient crack arrest test, the width of the test plate is \(W=300\) mm. Although the width of the specimen is a little bit less than the specified range of \(350\) mm \(\leq W \leq 1000\) mm (standard width: \(W=500\) mm) in the standard by JWES,\(^{11}\) the experimental result is expected to be useful for the validation of the proposed model as the first trial.

Figure 3 shows a configuration of the specimen. A test rig with 2 000 tonf capacity was used for pin-to-pin distance of 3 100 mm. A brittle crack was initiated by air-hammering the wedge attached to the notch with impact energy of 2.4 kJ, as recommended in the standard of JWES.\(^{11}\)

Applied stress was set as \(\sigma_{\text{app}}=177\) MPa. Temperature gradient near the arrested point was approximately \(dT/dx=0.55^\circ\text{C/mm}\) in the width direction, where \(x\) is a coordinate in the width direction. The results of temperature distribution are shown in Fig. 4.

Under the above conditions, the temperature gradient crack arrest test was conducted. Figure 5 shows fracture surfaces of the specimens after the arrest tests. It is found

| Thickness [mm] | Width [mm] | Position | Tensile test | V-notch Charpy test |
|---------------|------------|----------|--------------|---------------------|
| surf          | –          | –        | –            | –                   |
| 60            | 300        | t/4      | 464 [MPa]    | 552 [MPa]           |
|               |            | t/2      | 394 [MPa]    | 510 [MPa]           |
|               |            |          | EL [%]       | vTrs [°C]           |
|               |            |          | 30           | –63                 |
|               |            |          | –84          | –51                 |

Table 3. Mechanical properties in the rolling direction of the test steel.

Fig. 2. Distributions of equivalent circle diameter of the test steel. (Online version in color.)

Fig. 3. Configuration of the temperature gradient crack arrest test.

Fig. 4. Results of temperature distributions, arrested crack length and arrested crack temperature. (Online version in color.)
that 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. It is noted that there were not any theories which have quantitatively explained the formation of the split-nails in the past investigations.

Arrested crack length \( a \) was measured as the longest distance between the top of the specimen and the arrested crack front. The results of arrested crack length was determined as \( a = 154 \text{ mm} \), as shown as point plot in Fig. 4. In addition, the crack arrest temperature was determined as \( T = -9.2^\circ C \), based on the result in Fig. 4.

### 3.3. Model Simulation and Discussions

As described in the first part of the present paper, the proposed multiscale model as an integrated macroscopic model is performed by systematically integrating (1) a preparatory macroscopic finite element analysis and (2) a Monte Carlo simulation of microscopic analysis for cleavage fracture into (3) a macroscopic analysis for brittle crack propagation and arrest in steel plate. That is, the integrated macroscopic model is composed of the three-staged analyses. Therefore, the conditions and results of the respective stages of analyses are presented as follows.

It is noted that the brittle crack was initiated by the impact loading as described in Section 3.2. Considering the influence of the impact loading, the brittle crack behavior after the crack length of 60 mm was simulated in the present analysis.

#### 3.3.1. 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 \( r_c = 0.2 \text{ mm} \). \( \sigma_Y \) 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.

As the yielding condition of the dynamic finite element analysis, we employed the regression formula, expressed as

\[
\sigma_Y = \sigma_{Y0} \exp \left( \frac{(497.5 - 68.90 \ln \sigma_Y)}{T + 273} \frac{1}{18.42 - \ln \dot{\varepsilon}_0} \right) - \frac{1}{293} \] ........................ (2)

where \( \sigma_{Y0} \) [MPa] is yield stress at the room temperature, \( T \) [°C] is temperature and \( \dot{\varepsilon}_0 \) is equivalent strain rate. In addition, the true stress-strain curve is approximated by the Swift’s equation, expressed as

\[
\sigma = \sigma_Y \left( \frac{\dot{\varepsilon}_p + 1}{\alpha} \right)^n \] ........................ (3)

where \( \sigma \) is the von Mises stress and \( \dot{\varepsilon}_p \) is equivalent plastic strain. \( \alpha \) is a constant assumed as \( \alpha = 0.02 \). \( n \) is a strain hardening exponent and is assumed by the regression formula, expressed as

\[
n = -0.11097 + \frac{169.63}{\sigma_Y} - \frac{19580}{\sigma_Y^2} \] ........................ (4)

It is noted that \( \sigma_Y \) is obtained as the results of the finite element analysis because \( \dot{\varepsilon}_0 \) is obtained as the results of the analysis.

The nodal force release method is employed to simulate fast crack propagation. For simplification of the calculation, it is assumed that the crack surface is 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 \( V = 500 \text{ m/s} \) assuming just before crack arrest. For versatility, the width \( W \) and length \( L \) of the finite element model were determined so that the reflection of elastic wave at the boundaries did not interfere with the crack, as

\[
W > \left( 1 + \frac{V_R}{V} \right) a_{\text{max}} \] ................................ (5)

\[
L > \frac{V_R}{V} a_{\text{max}} \] ................................ (6)

where \( a_{\text{max}} \) is the maximum crack length (= 300 mm) and \( V_R \) is the elastic Rayleigh wave velocity. Figure 6 shows an example of the mesh of finite element model. One fourth model is employed due to symmetry. The minimum element size along a crack is 0.05 mm, which is smaller than the characteristic length of \( r_c = 0.2 \text{ mm} \) for the assurance of accuracy.

The distribution of temperature \( T \) was assumed as a linear function of \( x \) which has a gradient of \( \frac{dT}{dx} = 0.55 \text{°C/mm} \), as shown in Fig. 4. The remote applied stress is defined as \( \sigma_{sp} = 177 \text{ MPa} \), which is the same value of the experiment.

An example of the deformation and the maximum principal stress distribution obtained by the finite element analysis is shown in Fig. 7. The respective transitions of stress tensor \( \sigma \) at the mid-thickness, quarter-thickness and surface as the characteristic distance, i.e., \( r_c = 0.2 \text{ mm} \) from the crack tip are shown in Fig. 8. Only the normal components of stress tensor are shown in the figure because all the shear components are zero due to symmetry. The respective components of the stress tensor showed approximately linear decrease. Although all the stress components at the surface are the lowest compared with those at the mid-thickness.
of fracture surface \( n \) at the respective unit cell of the integrated macroscopic model. The details of the calculation procedures are shown in the first part of the present paper. 

The Monte Carlo simulation is performed for the microscopic analysis of cleavage fracture at the discrete evaluation points of the plate for efficiency of the whole analysis. In the present case, the number of evaluation points could be reduced due to the symmetry in the thickness direction (\( z \) direction). Therefore, nine discrete evaluation points are defined as respective three coordinates in \( x \) and \( z \) directions, i.e., \( x = 42 \text{ mm}, 114 \text{ mm} \) and \( 185 \text{ mm} \), which is correspond-

and quarter-thickness, they are little difference between at the mid-thickness and quarter-thickness. The respective yield stresses \( \sigma_y \) at the mid-thickness, quarter-thickness and surface at the characteristic distance from the crack tip is shown in Fig. 9. It is found that \( \sigma_y \) scarcely depends on the coordinate in the thickness direction.

3.3.2. Monte Carlo Simulation of Microscopic Analysis for Cleavage Fracture

The aim of the microscopic analysis for cleavage fracture is to calculate (1) fracture toughness \( k_{FM} \) and (2) direction of fracture surface \( n_M \) at the respective unit cell of the integrated macroscopic model. The details of the calculation procedures are shown in the first part of the present paper. 

The Monte Carlo simulation is performed for the microscopic analysis of cleavage fracture at the discrete evaluation points of the plate for efficiency of the whole analysis. In the present case, the number of evaluation points could be reduced due to the symmetry in the thickness direction (\( z \) direction). Therefore, nine discrete evaluation points are defined as respective three coordinates in \( x \) and \( z \) directions, i.e., \( x = 42 \text{ mm}, 114 \text{ mm} \) and \( 185 \text{ mm} \), which is correspond-
According to the temperature of $T = -70\, ^\circ C$, $-30\, ^\circ C$ and $10\, ^\circ C$, respectively, and, $z=0\, mm$, $15\, mm$ and $30\, mm$, which is corresponding to the mid-thickness, quarter-thickness and surface, respectively.

The required input data for the microscopic analysis is listed as (1) average grain size $d$, (2) distribution of grain orientation, (3) remote applied stress tensor $\sigma$ and (4) yield stress $\sigma_Y$. $d$ and the distribution of grain orientation are the characteristic parameters of steel plate as described in the above Section 3.1. $\sigma$ and $\sigma_Y$ are obtained by the preparatory macroscopic finite element analysis as shown in Section 3.2 and assumed as constants because the calculation domain is sufficiently small. In addition, two constants, which are the fracture toughness for cleavage fracture $k_{fm}$ and the critical shear strain to form tear-ridge $\epsilon_{fm}$, were assumed as $k_{fm} = 1\, MPa \sqrt{m}$ and $\epsilon_{fm} = 0.7$ in reference to the past study.

Trial number of the Monte Carlo simulation was set as 50 for the respective evaluation points. Examples of the obtained fracture surface in the microscopic analysis are shown in Fig. 10. The results of cumulative probability distributions (CPD) of the $k_M$ at each evaluation point are shown in Fig. 11. The results show that there is a large scatter even in the same evaluation point. The range of the scatter is generally larger than the difference between the averaged values of different evaluation points. The results also show that the average of $k_{fm}$ obtained in the mid-thickness is larger than those in the quarter-thickness and surface. In addition, it is clearly found that the lower temperature makes the larger $k_{fm}$. The reason can be explained as the dependence of yield stress on temperature. The results of the distributions of $n_M$ at each evaluation point are shown in Fig. 12. The results show that the largest scatter of the components of $n_M$ is found at the mid-thickness. On the other hand, the smallest scatter is found at the quarter thickness. Therefore, it is expect that the scatter of $n_M$ has a positive correlation with the strength of texture, as shown in Table 2.

### 3.3.3. Integrated Macroscopic Analysis by Model Synthesis

An integrated macroscopic analysis was performed to simulate the complicated brittle crack propagation and arrest behavior obtained by the experiments shown in Section 3.2.

The procedure in the integrated macroscopic analysis is composed of the two parts. The first part is the assignment
of the results of (1) stress tensor \( \sigma \), (2) yield stress \( \sigma_y \), (3) fracture toughness \( k_f \) and (4) direction of fracture surface \( n_M \) in each unit cell. \( \sigma \) and \( \sigma_y \) were obtained by (a) the preparatory macroscopic finite element analysis (see Figs. 8 and 9). On the other hand, \( k_f \) and \( n_M \) were obtained by (b) the Monte Carlo simulation of the microscopic analysis (see Figs. 11 and 12). The second part is the simulation of crack propagation and arrest in the macroscopic scale. The detail of the procedure is found in the first part of the present paper.

Based on the above conditions, the model simulation of crack propagation and arrest behavior by the integrated macroscopic analysis was conducted. The simulation results of the transition of fracture surface morphology are shown in Fig. 13. The arrested crack length in the simulation result was \( a = 158 \) mm. Therefore, the proposed model accurately simulated the arrested crack length in the experimental result of \( a = 154 \) mm. The result shows that the crack was arrested, although arrest toughness is decreased with the crack propagation as shown in Fig. 11. The reason can be approximately explained by the fact that the decreasing rate of the arrest toughness according to the crack propagation is less than that of the local stress as shown in Fig. 8.

For detail of the simulation results, although the shape of the crack front was approximately straight in the initial stage, the crack propagation near the mid-thickness was gradually delayed. As a result, a “split nails” \(^{23}\), where the crack front at the quarter-thickness is advanced to the crack propagation direction, was presented at the arrested point. Figure 14 shows a comparison between experimental and simulation results of the fracture surfaces in the \( xz \) view. The tendency of the shape of arrested crack front in the simulation result shows good agreement with that of the experiment result. In particular, the formation of the split nails was successfully simulated with accuracy. The boundaries of unit cells, which have the gaps of larger than 1 mm and 2 mm in average, are also shown in Fig. 14 in blue and red, respectively. The boundaries shown in red and blue in Fig. 14 represented a globally good tendency of the “chevron pattern” in the fracture surface obtained by the experiment. One of the differences between the experimental and simulation results is a formation of the shear-lips near the plate surface. The shear-lip formation is a characteristic ductile fracture surface formed by the relaxation of plastic constraint near the surface\(^{24}\) and is not considered in the proposed model. Although the modeling and implementa-
tion of the shear-lip formation may be one of the future consideration, the influence is expected to be sufficiently small on the entire phenomenon.

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

4. Conclusion

In the present paper, we proposed a new multiscale model by a “model synthesis” approach, as the first attempt to clarify the relationship between microstructures and macroscopic brittle crack propagation/arrest behavior in steel plate.

As described in the first part of the present paper, the proposed multiscale model as an integrated macroscopic model is performed by systematically integrating (1) a preparatory macroscopic finite element analysis and (2) a Monte Carlo simulation of microscopic analysis for cleavage fracture into (3) a macroscopic analysis for brittle crack propagation and arrest in steel plate. That is, the integrated macroscopic model is composed of the three-staged analyses.

The second part of the present paper showed an applica-
tive components of crack tip showed approximately linear decrease. The repre-
pared with those at the mid-thickness and quarter-thickness. On the other hand, the direction of fracture surface makes the larger scatter of $k_M$ obtained in the mid-thickness was the largest compared with those in the quarter-thickness and surface. In addition, it is found that the lower temperature direction as follows.

The procedure in the integrated macroscopic analysis, which is the third stage of analysis, is composed of the two parts: (a) the assignment of $\sigma$, $\sigma_m$, $k_M$ and $n_M$, which were obtained in the previous analyses in each unit cell, and (b) the simulation of brittle crack propagation and arrest behavior in the macroscopic scale. As a result, the proposed multiscale model successfully simulated the complicated brittle crack propagation and arrest behavior for the steel plate having nonhomogeneous distributions of microstructures in the thickness direction. In particular, the followings are the typical achievements in the integrated macroscopic analysis: (1) the arrested crack length was well simulated with high accuracy; (2) the “split nails”, where the crack front at the quarter-thickness is advanced to the crack propagation direction, was accurately simulated; (3) a globally tendency of the “chevron pattern” of the fracture surface was well represented. It is therefore found that the proposed model has been validated in spite of complicated phenomena from the results of the comparison between proposed model and experiments.

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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