1. Introduction

Prevention of brittle fracture is crucially important in securing reliability of welded steel structures like ship-hulls, cryogenic storage tanks and pressure vessels. For these structures, the double integrity concept is applied, in which initiation of brittle fracture at welds is prevented but at the same time the initiated and propagating crack is controlled to arrest at base metal. To realize the latter, steel plates having high crack arrest toughness must be used in the structures. For example, recent rapid increase of container ship hull size has necessitated the use of very thick high-strength steel plates, as thick as 80 mm or more, and crack arrest toughness is required for these steel plates by ship classification societies. Recently, sophisticated thermo-mechanical control process (TMCP) is applied to realize high crack arrest toughness as well as high strength through grain-refinement in such thick plates1,2. It is well known that grain-refinement of steel improves toughness but generally microstructural effects on the crack initiation and arrest toughness is not all the same3.

It is well known, on the other hand, that brittle fracture surfaces of steel plates exhibit irregularities with typical morphology, known as chevron markings or herring bone patterns4-8. Figure 1 shows an example of the chevron markings on brittle fracture surface of 30 mm thick mild steel weld. Many attempts have been made to understand the cause of fracture surface irregularities. Kies et al.4 and Boyd5 explained the reason of the chevron markings as centrally concentrated crack initiations leading but scalloped crack front. Tipper6 and Carlsson7 attributed the cause of the chevron markings by initiation of internal (subsidiary) cracks connecting the main crack. Gash8 classified the morphologies of brittle fracture surfaces and discussed the cause of chevron markings based on the reflection of stress wave. It might generally be recognized that brittle fracture surface is smooth at lower temperature and rough and irregular at higher temperature, often associated with deep chevron markings in the latter. It also seems that the formation of the chevron markings depends on microstructures of steels, as well as testing conditions.

Numerical simulation and experiment on brittle fracture surface morphologies in steel*

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A numerical simulation model of brittle crack propagation was developed incorporating fracture surface irregularity, and small-scale crack arrest experiment of a steel plate was conducted to validate the model. Mechanisms of the formation of brittle fracture surface irregularities including chevron markings in the steel were discussed based on the model calculations and the experiment. Formation of the chevron markings was found to depend on applied stress intensity factor. The model calculations and the experiment showed that the chevron markings are nucleation and continuation of ridges, which are formed between two cleavage crack terraces with different height levels. The dependence of the extent of the chevron markings on applied stress intensity factor is understood as that a deep ridge reduces local stress intensity factor by shear stress acting on the ridge, and the deep ridge can develop only at high stress intensity factor level but only shallow ridges are possible if stress intensity factor level is low. This tendency agreed between the experiment and the calculation. Relationship between crack arrest toughness and fracture surface irregularities is discussed.

Key Words: crack propagation and arrest, brittle fracture, cleavage fracture, steel, fracture mechanics, fractography, numerical simulation

Fig. 1 Example of chevron markings, mild steel weld.
surface irregularities into account are not many. One of its reasons might be that the standard fracture mechanics, which assumes a flat crack, cannot directly be applied to irregular cracks. Melinteck proposed a computer simulation model to reproduce irregular brittle fracture surface at grain-size level. Following his study, Qiao and Argon proposed a more sophisticated model, in which non-uniform cleavage crack propagation in polycrystalline steel microstructure was modeled and compared with observed fracture surface at microscopic level. One of the present authors proposed a numerical simulation model of crack propagation in bcc polycrystalline solids. They carefully observed cleavage fracture surface of steel and microscopic crack propagation directions and found that the crack propagation is essentially continuous from grain to grain but the crack propagation directions become different at some point and the difference in the directions increases gradually with crack advance and finally a step or a ridge between the cleavage crack planes is formed at grain-size level. Similar result was noticed in. Shibanuma et al. and Yamamoto et al. extended the study of to macroscopic brittle crack propagation.

In spite of the above-mentioned studies, the mechanism of brittle fracture surface formation, including the chevron markings, is far from complete understanding, nor have conditions of the chevron marking formation been clarified. The present study aims at proposing a mechanism of fracture surface formation with irregularities by using a newly developed numerical simulation model and observing brittle fracture surfaces of crack arrest test of a steel plate. Relationship between fracture surface irregularities and crack arrest toughness is also discussed. Here, brittle fracture in steels is associated with cleavage fracture in the present study. Therefore, the present study deals with cleavage crack propagation.

2. Numerical Modelling

One of the authors proposed a numerical model to simulate cleavage crack propagation in bcc polycrystalline solids, in which crystal grains were modelled as columnar cells, a flat crack was assumed in each cell and overall fracture surface was constructed as an aggregate of the flat cracks. The proposed model is extended in the present study. To determine a flat crack in each cell, three \{100\} planes, having a right angle each other, were assumed randomly. For a cell in front of a crack-tip, normal stress acting on each \{100\} plane is calculated from local stress intensity factors of the mixed mode, \(K_{IJ}^{tip}, K_{II}^{tip}, K_{III}^{tip}\), and the plane having the maximum normal stress is selected as a cleavage plane, see Fig. 2. Because the constructed fracture surface is not flat nor is the crack front straight, it is a laborious task to calculate \(K_{IJ}^{tip}, K_{II}^{tip}, K_{III}^{tip}\) for such an irregular crack, accurately. Therefore, approximate formulae were applied to do so. To take the influence of crack front non-straightness, equation developed by Rice was applied, Fig. 3.

\[
K_{non-straight}(z) = K^\infty [z; a(z)] + \frac{1}{2\pi} P.V. \int_0^z \frac{K^\infty [z'; a(z')] [a(z') - a(z)]}{(z' - z)^2} dz'
\] (1)

where, \(a(z)\) represents crack front shape, \(P.V.\) stands for Cauchy principal value of the integration and \(K^\infty [z]\) is distribution of stress intensity factor along straight crack front. Also, equations developed by Gao was applied to take account of the fracture surface irregularity, Fig. 4. His analysis is an extension of the analysis for two-dimensional curved crack developed by Cotterell.

\[\text{Fig. 2 Determination of cleavage crack plane in front of crack front, numerical model.}\]

\[\text{Fig. 3 Schematic of non-straight crack front, numerical model.}\]

\[\text{Fig. 4 Schematic of fracture surface irregularity, numerical model.}\]
In the present study, tilt and twist of the crack surface at crack-tip is influential. These stress intensity factor calculations are based on the first order approximation and all the effects of crack surface irregularities are linearly superposed to calculate the mixed mode stress intensity factors. The constructed fracture surface is not continuous because there is a ridge between adjacent cells due to twist and tilt. Ridges are formed also because cracks having propagated from different directions meet each other and there can be a step or ridge between the cracks, see Fig. 5. The ridge between the cells carry shear stress having an effect of crack closure. Because the ridge is expected to shear-yield just after the crack-front passes through this point, the shear stress acting on the ridge can be assumed equal to the shear-yield stress of the material. This effect is taken into consideration in the present model. As explained above, the present model assumes a single and continuous (not discrete) crack which has non-flat crack surface and non-straight crack front. It is also assumed that the crack closing forces are applied on the crack faces. These simplifications enable to calculate local stress intensity factors along the crack front, without relying on a finite-element analysis. Local cleavage fracture criterion is incorporated, i.e., cleavage fracture is assumed to extend in a cell if local stress intensity factor, $K_{eq-normal}$, exceeds local fracture toughness, $K_{c-local}$,

$$K_{eq-normal} \geq K_{c-local}$$  \hspace{1cm} (2)

$K_{eq-normal}$ represents a magnitude of the normal stress acting on the selected plane and is calculated as,

$$K_{eq-normal} = n_i^m \sum_{a=1}^{3} \left(K_a^{tip} f_i^a(\theta_m) \right) n_j^m$$  \hspace{1cm} (3)

where $n_i^m$ is normal vector of the $m$-th {100} plane, $K_a^{tip}$ is local stress intensity factor of the $a$-th mode and $f_i^a(\theta_m)$ is a function expressing stress tensor near a crack-tip in linear elastic solid and $\theta_m$ is angle of the $m$-th {100} plane relative to the $x$-$z$ plane ($m = 1, 2, 3$). $K_a^{tip}$ reflects the influences of the crack surface irregularity, crack front non-straightness and shear stress acting on the ridges. On the other hand, $K_{c-local}$ represents a resistance of the material against cleavage fracture and may be related to the cleavage fracture stress of bcc lattice. Because the grains are assumed as columnar cells, cleavage crack extension is treated in a discrete and step-wise manner, see Fig. 6. A crack may extend across grain boundary at an edge of a cell (Active front) but it may not at a different edge ( Arrest front). Fracture surfaces constructed by the model were well compared with experimentally observed fracture surfaces on a grain-size level.

In the present study, the model proposed by is extended to macroscopic fracture process. In their model, the crystal grains are modeled by columnar cells but a cell in the present model has a size much larger than the grain size, typically, 0.25 mm. In this case, the cell contains many grains and {100} planes can no more be assumed and the cleavage crack is not flat at all in the cell. However, we assume that directions of the cleavage cracks in a cell are not random but they concentrate on a certain direction because maximum principal stress direction might be assumed nearly the same in a cell and therefore cleavage planes in the cell are selected so that they are as close as normal to the maximum principal stress, see Fig. 7. Then, we assume that the algorithm employed in can be applied at macroscopic level. Therefore, the cell is “pseudo” crystal grain and the crack plane in the cell is “pseudo” cleavage crack in the present model.

We employed further assumptions for simulating macroscopic fracture. $K_{c-local}$ in Eq.(2) should be regarded as crack propagation resistance of a material and it should be related to microscopic and
metallurgical factors including grain size, temperature and possibly crack velocity. But, we assume that $K_{c-local}$ is related to macroscopic crack arrest toughness, $K_{ca}$, as,

$$K_{c-local} = \alpha_K K_{ca} \tag{4}$$

where, $\alpha_K$ is a constant. $K_{ca}$ may be determined by crack arrest test \(^{18}\), but we assume that $K_{ca}$ is expressed by an empirical formula, as a function of Charpy impact test absorbed energy transition temperature, $vT_{re}$, plate thickness, $t$, and temperature, $T$, \(^{19}\),

$$K_{ca}[\text{MPa}\sqrt{\text{m}}] = 480 \exp\left[103.349+0.00691 vT_{re}[\text{deg.C}] + 0.0055 (\text{mm}) \right] \cdot \left[0.0327 - 1/\sqrt{T[K]} \right]. \tag{5}$$

Figure 8 shows a calculated result of $K_{ca}$ for $t=30$ mm and $vT_{re}= -20, -40$ and $-60$ deg.C. Using Eq. (3) and Eq. (4), $K_{c-local}$ is expressed by $vT_{re}$, $t$ and $T$. Although, this representation has been derived via $K_{ca}$, $K_{c-local}$ is expressed using Charpy impact property, which might represent the effect of microscopic and metallurgical factors on crack propagation resistance.

As has been mentioned previously, a brittle crack near the mid-thickness of a steel plate precedes that near the plate surfaces, so-called crack tunneling. Reason for this is understood as that plane strain condition is maintained near the mid-thickness while it is lost near the plate surfaces so the crack propagation is retarded near the plate surfaces. At very near the plate surfaces it is no more possible for the crack to propagate in a brittle manner; uncracked ligaments are formed and they are fractured in ductile manner to form shear-lips on fracture surface. This phenomenon was modelled by Shibanuma et al. \(^{20,21}\). They assumed that a depth of the zone where the plane strain condition is lost is equal to $(1/3\pi)(K_d/\sigma_Y)^2$, where $K_d$ is dynamic stress intensity factor and $\sigma_Y$ is yield stress of the material with strain-rate effect incorporated. Furthermore, they assumed that brittle fracture does not take place within this zone. Their model reproduced actual brittle fracture surface with shear-lips and crack-tunneling, accurately. Although this phenomenon is a consequence of the loss of the plane strain condition near the plate surfaces, this can be replaced by the increase in crack arrest toughness there. Hence, in the present model, $K_{ca}$ is assumed to have a distribution in the thickness direction but it depends on the magnitude of stress intensity factor, as shown in Fig.9. Note that static stress intensity factor is used in the present study for simplicity. Random “pseudo” \{100\} planes are assigned in each cell and a “pseudo” cleavage plane is selected in the cells according to the above-mentioned algorithm. After this step is complete, shape of a new fracture surface is constructed along the crack front, mixed mode stress intensity factors are calculated along the newly formed crack front and new fracture surfaces are determined in the next step. If cleavage fracture no more takes place at all along the crack front, then the crack is judged to be arrest and the calculation is finished. As has been explained above, the present model is quasi-static and does not include dynamic (inertial) effect associated with crack propagation.

### 3. Experimental

The aim of the present experiment is to observe cleavage fracture surfaces of crack arrest test specimens of steel, to validate the numerical model and to identify influencing factors on the fracture surface morphologies.

#### 3.1 Experimental procedures

Tested steel, whose chemical composition is 0.14%C - 0.41%Si - 1.45%Mn - 0.017%P - 0.003%S (mass%), was produced by normalizing heat treatment following hot rolling. Therefore, its microstructure is equi-axed ferrite-pearlite, as shown in Fig.10. Practically random crystallographic orientation can be expected. Table 1 shows mechanical properties.

Coupins with 12.7 mm thickness (thickness reduced), 76 mm width and 305 mm length were machined from the steel in the longitudinal direction and they were press-notched by pressing a chisel on the specimen side face at ambient temperature so as to
produce a 5 mm or 10 mm deep notch, as shown in Fig. 11. Subsequently, the press-notched specimens were subjected to bend-test, according to the testing procedure described in WES-TS 2816 and Kawabata et al. Specimen temperature was controlled by setting the specimen in a cooling bath filled with alcohol, which was cooled by liquid nitrogen. Specimen temperature was monitored by thermo-couples attached near the notch-tip and specimen bottom. The specimen was quasi-statically loaded through three-point-bend jig. Load at brittle fracture initiation was recorded. Subsequently, the load was relieved and the specimen was cooled to liquid nitrogen temperature and re-loaded to break the specimen into two for observing fracture surfaces.

Crack arrest toughness, $K_{ca-PB}$, was calculated using the following formula.

$$K_{ca-PB} = \frac{3P}{2BW^2} \sqrt{\frac{a_0}{W}} \left[ 1 + \frac{18\pi}{5}\left(\frac{a_0}{W}+6v(\xi_0)\right) \int_{\xi_0}^{\xi_A} F(\xi) \frac{d}{d\xi} \right]^{-\frac{1}{2}}$$

where, $P$ is load at brittle fracture initiation, $B$ is specimen thickness, $W$ is specimen width and $S$ is bending span, see Fig. 11. $\xi = a/W$, $\xi_0 = a_0/W$ and $\xi_A = a_A/W$, where $a_0$ is notch depth but it includes ductile crack length if observed at a notch-root and $a_A$ is average arrest crack length measured on the fracture surface, including the initial notch. Functions $V(\xi)$ and $F(\xi)$ are expressed as,

$$V(\xi) = \left(\frac{1}{\xi_0}\right)^2 \left(12.77\xi^4 - 34.94\xi^3 + 36.82\xi^2 - 19.57\xi + 5.58\right)$$

$$F(\xi) = \frac{1.99 ((1-\xi)(2.7\xi^2+3.93\xi+2.15))}{\sqrt{1-(1-\xi)^{2/3}(2\xi+1)}}$$

Eq.(6) was derived by assuming fixed displacement condition during crack propagation until crack arrest. Fracture surfaces were photographed and macroscopically observed after the test.

### 3.2 Experimental result

Totally 12 tests were conducted. Figure 12 shows a summary of the test result. Transition behavior of the crack arrest toughness was obtained. It is noted that 2 tests did not satisfy the validity criterion because $a_A$ was longer the upper limit. Four specimens were selected for detail fracture surface observation and numerical simulation, as shown by the red plots in the figure.

Figure 13 shows changes of stress intensity factor during crack propagation for the selected specimens, but in this case instantaneous crack length was inserted in Eq. (6), instead of arrest crack length.
Note that $a_0 = 5$ mm for the specimen N25 and N32 and $a_0 = 10$ mm for N37. It is also noted that ductile crack extension was observed in the specimen N36 so $a_0 = 13$ mm, including 10 mm deep pressed notch and 3 mm deep ductile crack, see Fig. 14(c). Brittle fracture initiation load was 130 to 156 kN, independently of the test temperature probably because compressive residual stress might have been induced at the notch-tip by press-notching.

Figures 14(a) to (d) show fracture surfaces of the selected specimens. Red arrows indicate crack arrest position. In case a brittle crack re-initiation was observed, initial crack arrest point was selected and used for calculating the crack arrest toughness. Crack tunneling and shear-lips were found more pronounced at higher temperature. Chevron markings were evident in all the specimens but they were not uniform along the crack path, especially in the specimen N36 ($-50^\circ$C) and N37 ($-60^\circ$C), that is, the chevron markings were clear from the notch-root to the half way of crack propagation but they tended to disappear in the latter half. It is obvious from the present experiment that the fracture surface irregularity is not uniform even at the same temperature but it depends on other parameters, as well.

### 4. Numerical Model Calculations

The proposed model has been applied to the press-notched bend test presented in the previous section. Table 2 shows parameter values assumed in the calculations. The cell size was 0.25 mm, considering a computer capacity. Fifty cells were allocated in the thickness direction to realize 12.5 mm specimen thickness, which enables minimal resolution of the fracture surface morphology. Thickness difference between experiment and calculation is

| Table 2 Conditions for Numerical Simulation |
|---------------------------------------------|
| Cell size | 0.25mm |
| Specimen Thickness | 12.5mm (50 cells) |
| Specimen Configuration | notched three-point bend |
| Yield Stress (tear-ridge, plastic zone size) | 800MPa |
| Temp. Distribution | isothermal (-20$\text{ to } -60^\circ$C) |
| Local toughness parameter, $a_K$ | 0.2 |
| Plate surface toughness parameter, $\delta_c$ | 5 |

Fig. 14 Fracture surfaces, (a) N25: $-20^\circ$C, $a_0 = 5$ mm, $P_0 = 156$ kN, $a_A = 37$ mm, (b) N32: $-40^\circ$C, $a_0 = 5$ mm, $P_0 = 142$ kN, $a_A = 50$ mm, (c) N36: $-50^\circ$C, $a_0 = 13$ mm, $P_0 = 156$ kN, $a_A = 71$ mm, (d) N37: $-60^\circ$C, $a_0 = 10$ mm, $P_0 = 130$ kN, $a_A = 73$ mm. Intervals of length scale is 10 mm.
negligible. Yield stress was assumed as 800 MPa, accounting for its increase by high strain-rate near a propagating crack-tip. Temperature effect on yield stress was not considered due to relatively narrow temperature range, -60 to -20 deg.C. Shear yield stress was assumed equal to the half of the yield stress, assuming Tresca yield criterion. To determine the value of $\alpha_K$, the present model was preliminarily applied to a hypothetical temperature-gradient crack arrest test\(^\text{18}\), assuming a distribution of $K_c(a)$ using Eq.(5) from temperature distribution in the specimen width direction and assuming a value of $\alpha_K$, arrest crack length $a_A$ was determined from the model calculation. The value of $\alpha_K$ was determined by a trial-and-error so that the value of $a_A$ agreed with the arrest crack length determined from the equation, $K_c(a) = \sigma \sqrt{\pi a}$ (Eq.(5)). Several calculations were conducted by changing applied stress $\sigma$ and temperature distribution and finally the value of $\alpha_K$ was determined as 0.2 by averaging the obtained values\(^\text{19}\). It should further be noted that $K_{c-local}$ should be independent of the specimen thickness (thickness effect on arrest toughness). Therefore, a constant value, $t=50$ mm, was used in Eq.(5), regardless of the specimen thickness. Value of $\alpha_c$ was assumed equal to 5, tentatively. In the model calculations of the press-notched bend test, change of static stress intensity factor with crack length followed that of Fig.13. The initial crack was assumed to be straight, regardless of the ductile crack extension prior to the brittle fracture. A bowing crack front, simulating the ductile crack extension, was possible but was not employed here because it might not influence the overall crack surface morphology.

Figure 15(a) to (d) show calculated fracture surfaces, corresponding to Figs. 14(a) to (d). Color indicates height ($y$-coordinate) of the fracture surface for clarity. As temperature decreased, arrest crack length became longer, except for the specimen N37. This tendency agreed with the experiment. Shorter arrest crack length in the specimen N37 than in the specimen N36 might be because the fracture initiation load was lower in the former. Also, the assumed stress intensity factor value might be less accurate at longer crack length, especially at short ligament length, because the present model is quasi-static under fixed displacement condition. It should be noted that crack front tunneling in the model calculation was more pronounced at higher temperature, which agreed well with the experimental result. An interesting result in the present numerical simulation is that the chevron markings were reproduced without any additional algorithm, \textit{i.e.},

![Fig. 15](image-url)

(a) N25: -20°C, $a_0=5$ mm, $P=156$ kN, $a_A=37.5$ mm, (b) N32: -40°C, $a_0=5$ mm, $P=142$ kN, $a_A=47.5$ mm, (c) N36: -50°C, $a_0=13$ mm, $P=156$ kN, $a_A=64.8$ mm, (d) N37: -60°C, $a_0=10$ mm, $P=130$ kN, $a_A=59.8$ mm.

Intervals of length scale is 10 mm.
ridges were spreading from the mid-thickness towards specimen surfaces. More interestingly, extent of the chevron markings changed with crack length. This tendency is most clearly recognized in the specimen N36, see Fig. 15 (c), in which the chevron markings were relatively clear and deep until the crack propagated to about 50 mm and tended to disappear at longer crack length. This can be compared well with the experiment, Fig. 14 (c), in which the chevron markings were clearly observed until the crack propagated to about 50 mm and tended to disappear at longer crack length. As recognized in Fig. 13, the stress intensity factor in the numerical simulation decreased with increasing crack length except at very short crack length. The present numerical simulation result strongly suggests that the occurrence of the chevron markings is strongly influenced by the magnitude of stress intensity factor rather than other effects, e.g., dynamic effect or crack velocity. To verify this notion, additional calculation was conducted for the specimen N36 but in the present case stress intensity factor was kept constant at 150 MPa√m. Result is shown in Fig. 16. Because the crack was not arrested in this calculation, the crack up to 80 mm is shown. Evidently, the chevron markings appeared on the entire fracture surface. This result supports the above notion. It is noted that temperature effect on the extent of the chevron markings was not clear both in the experiment and the calculations within the temperature range investigated. It should be mentioned that plastic deformation prior to the crack propagation may influence the fracture surface morphology, especially near the notch-root. However, the influence of the plastic deformation alone cannot explain the change of the fracture morphology because general yielding was not observed in the specimens.

To understand the role of the magnitude of stress intensity factor on the formation of chevron markings, detailed observations were made for the calculated fracture surface of the specimen N36. Figure 17 is the same figure as Fig. 15 (c) but red boxes are indicated, in which detailed observations were made. Firstly, Fig. 18 shows crack propagation directions in each cell in the box “1”, in which a chevron marking line was nucleated. At point “A”, the cleavage crack began to propagate at different (lower and upper) directions, forming lower terrace “a” and upper terrace “b”. Then the ridge “r1” developed between the two terraces. The lower terrace “a” propagated between two upper terraces “b” and “c” and the ridge depth increased with increasing distance from point “A”. Cleavage cracks were frequently arrested near the ridge “r1”, as indicated by red arrows and a crack of the neighbor propagated further. As a result, the ridge gradually changed its direction, toward the specimen surface. Evidently, a chevron marking line is a continuation of the ridge.

Next, deep and shallow chevron markings were compared in the box “2” and “3” in Fig. 17. Figure 19 shows how the ridge developed with calculation steps in the box “2”. Cleavage crack was arrested at point “A” (step: 128) but cleavage fracture continued to propagate at point “B” (step: 129). The crack “C” was arrested (step: 130) but fracture continued to propagate at point “D”
This sequence continued and the ridge “r” developed in diagonal direction. The same process continued at the lower terrace, point “E” and “F”, etc. Figure 20 shows close-up view of the box “3” in Fig. 17. The cleavage crack was arrested at point “A” (step:258) but a sequential process like that in the box “2” did not continue; i.e., cleavage cracks developed at point “B” at upper terrace and point “C” at lower terrace (step:259 to 262) and the both cracks joined together (step:263). At this point, the ridge “r” was terminated.

To show the crack-closure effect by the ridges between the cells (Fig.5) quantitatively and understand the difference in the continuation and termination of the ridges in Fig.19 and 20, respectively, distributions of stress intensity factors were compared with instantaneous crack shape, see Fig.21 (a) and (b). Average crack length of Fig.21 (a) and (b) was 38.9 mm and 59.3 mm and the crack front contains the box “2” and “3”, respectively. Green line indicates a distribution of mode-I stress intensity factor, $K_I$, accounting for the non-straight crack front and red line indicates a distribution of mode-I stress intensity factor, $K_{I-ridge}$, which is associated with shear stress acting on the ridges, i.e. it has a crack closure effect, see Fig.5. Black line is a net stress intensity factor, $K_{In}=K_I-K_{I-ridge}$. Not that a small discrepancy between the value calculated by the equation and that shown in the figure is due to moving average effect. Also note that average $K_I$ values for the both crack lengths are 128 MPa$\sqrt{m}$ and 76 MPa$\sqrt{m}$, respectively, see Fig.13. Steep rise of $K_{I-ridge}$ is observed at deep ridges indicated by red arrows in Fig.21 (a). Therefore, $K_{In}$ is reduced there. But, it is still higher than $K_{c-local}$, as indicated by dotted line, because $K_I$ is high at this crack length (Change of $K_{c-local}$ in the thickness direction is small because the uncracked ligaments
develop little.). On the other hand in Fig. 21 (b), $K_I$ is lower than that of Fig. 21 (a) and the fracture condition, Eq. (2), is satisfied only if $K_{I-ridge}$ is low corresponding to shallow ridges. This might be the reason why deep chevron markings were realized at high stress intensity factor, more exactly excess stress intensity factor $K_{I-ridge}$ and they tended to disappear at low stress intensity factor both in the experiment and numerical simulation. In other words, a crack can propagate with deep ridges if stress intensity factor is sufficiently high, but only shallow ridges are possible for a crack to propagate at low stress intensity factor. It should be noted that the present numerical model is purely quasi-static and the crack velocity effect cannot be discussed quantitatively. But, excess stress intensity, $K_{I-n}-K_{c-local}$, might be converted to kinetic energy, thereby increasing crack velocity. The case in Fig. 21 (b) shows almost balanced values between $K_{I-n}$ and $K_{c-local}$, probably corresponding to lower crack velocity. In fact, it was just before crack arrest in this case.

Next, crack propagation behavior just before crack arrest was compared between the specimen N36 (~50°C) and N25 (~20°C), see Figs.22 and 23, respectively. As was shown in Figs.14 and 15, the crack tunneling was more pronounced in the specimen N25. While the crack front was straighter in the specimen N36, it was bowing in the specimen N25. But, more interesting point in the latter specimen is that a crack was partially arrested near the specimen surfaces and the crack front became partially inactive prior to the complete crack arrest; the crack arrest was not at once but gradual. The inactive crack fronts extended towards the mid-thickness. As a result, crack tunneling became more pronounced. It should be noted that the crack did not propagate with the same shape of the tunneling front at arrest but the crack front became more bowing because the inactive crack front became deeper. It is also noted that the chevron marking lines did not always have a right angle with crack front.

5. Discussion

Kies et al.⁴ and Tipper⁶ discussed the mechanisms of chevron markings and they concluded that an isolated crack is initiated ahead of a main crack and the initiated and the main crack are joined up and the ridges are formed due to a level difference between the both cracks. The present numerical model succeeded in reproducing the chevron markings without assuming isolated crack initiation ahead of a main crack. Also, it was observed¹⁵ that most of the cleavage cracks were continuous from grain to grain and isolated crack initiation sites were seldom observed on actual cleavage fracture surface of steel. Generally, subsidiary cracks are often observed under a main crack. But, it was confirmed by successive sectioning of a sample that these cracks were continuous with the main crack; these were not isolated but branched from the main crack²⁴. These observations support the mechanism of the chevron marking formation proposed in the present study, i.e., a chevron marking is a nucleation and continuation of a ridge. As was shown in Fig. 18, a crack happens to propagate at different (lower and upper) directions and a ridge is nucleated between the two terraces. As the crack propagates, the ridge becomes deeper if crack propagation with the different directions continues. When the ridge becomes deeper, local stress intensity factor decreases due to crack closure force acting on the unbroken ridge, where shear stress equal to shear yield stress is expected to exert. If applied stress intensity factor is sufficiently high, crack can continue to propagate even if the ridge is deep and the crack closure force is high; the chevron marking continues to
develop. But, if applied stress intensity factor is not sufficiently high, the crack is arrested near the ridge; the chevron marking is terminated. The present model has shown that the chevron markings develop more at higher stress intensity factor. This was reasoned by the distributions of stress intensity factors, as shown in Fig. 21.

To validate the present model and the above hypothesis, detailed observation was made for an actual brittle fracture surface, additionally. The same steel (30 mm) as Table 1 was subjected to temperature-gradient crack arrest test using a wide plate specimen with 500 mm width, complying with the test method WES 2815 (2014). Applied stress was 300 MPa and temperature at crack arrest was -6°C. Fracture surface was observed within about 100 mm from the arrest position using 3D laser scope, KEYENCE One-Shot 3D Measurement VR-3000/3200. Figure 24 shows the result. Many ridges are observed. For example, at point “A”, the crack began to propagate into different directions and the ridge “r1” was formed. There is no indication of isolated crack initiation around the point “A”. The ridge continued to develop until it propagated near to the specimen surface point “B”; a chevron marking was formed. At point “C”, on the other hand, the crack began to propagate into different directions to form the ridge “r2”. The ridge did not propagate at long distance but the separated crack (two terraces) merged at point “D”. Similarly, a short ridge “r3” was observed but in this case it is clearly seen that the upper terrace was arrested (point “F”) and a crack detoured around the point “F” to merge into one. There are many short and long ridges on the fracture surface. Overall, the fracture surface morphologies constructed by the present model agree with the experimentally observed ones well.

Termination of the ridge by merging of the upper and lower terraces may be stochastic because the propagation directions of the terraces are stochastic. But, sufficiently high stress intensity factor is a necessary condition for a ridge to continue to develop because local stress intensity factor is reduced by the shear force acting on the ridge. At low stress intensity factor, deep ridges cannot develop at long distance. That is a main reason why the extent of the chevron markings changed with crack length even at a constant test temperature, Figs. 14 (c) and (d).

To validate this mechanism furthermore, a numerical calculation was conducted for a temperature-gradient crack arrest test. The test identical as Fig. 24 was chosen. As additional information, temperature gradient was 0.3°C/mm in the specimen width direction and the temperature at specimen width center was -6°C. Initial notch length was 29 mm. Crack resistance was assumed the same as Fig. 8 with Charpy transition temperature of -40°C. Temperature dependence of yield stress was not considered for simplicity. Sixty cells with a size of 0.5 mm was allocated in the thickness direction to model the 30 mm thick plate. The values as same as those in Table 2 were used. Stress intensity factor was assumed as $K = \sigma \sqrt{\pi a}$. Figure 25 shows calculated result with experimentally observed fracture surface of the same testing condition. Calculated arrest crack length was 309 mm, as compared with the experimental value of 302 mm. Many chevron markings appeared on the fracture surface.
calculated fracture surface. Interestingly, the crack was smoother from the notch root to about 100 mm and the chevron markings became clearer at longer crack length. This tendency agrees with the experimentally observed fracture surface. This tendency was opposite with the press-notched bend test; the stress intensity factor increases in the temperature-gradient crack arrest test, as shown in Fig. 26, as opposed to the press-notched bend test. Therefore, the present result is reasonable. It should further be mentioned that the experimental fracture surface was most irregular at crack length of about 120 mm to 220 mm. At this crack length range, gap between $K$ and $K_{ca}$ is relatively large. This point might support the hypothesis proposed by the present study. The calculated fracture surface exhibits the same tendency with the experiment. Not complete agreement on the position of the deep chevron markings between the simulation and the experiment might be because the present model is based on the quasi-static calculation. Further improvement of the model incorporating the dynamic effect must be necessary for more accurate calculations.

Influence of temperature on brittle fracture surface irregularities has not been clarified in the present model. Generally, the brittle fracture surface is more irregular at higher temperature and flatter at lower temperature, as shown in Fig. 25. Crack arrest tests are often conducted at low applied stress (low stress intensity factor) at lower temperature. The present model infers that low stress intensity factor is one the factors on the formation of the flatter fracture surfaces at lower temperature. If there is an excess energy at lower temperature, it might be converted to kinetic energy promoting higher crack velocity rather than enhancing chevron markings because it is easier for a crack to realize high crack velocity due to smaller plastic deformation at crack-tip with higher yield stress at lower temperature. If the excess energy is too much to be converted to kinetic energy, crack branching might occur. On the other hand, higher stress is often applied at higher temperature to realize a certain crack propagation length. In that case, the stress intensity factor is excessive and the excessive energy might be consumed by more irregular fracture surfaces having deep ridges rather than consuming it by kinetic energy.

Although, the fracture surface morphology was well reproduced in the present model, formation of the uncracked ligament was not accurately reproduced; compare Fig. 14(a) and Fig. 15(a), and also Fig. 25. Formation of the uncracked ligament was modelled by taking the decrease in the plastic constraint near the specimen surfaces into account in the present model. However, crack-closing forces exert on the uncracked ligament, thereby decreasing the effective stress intensity factor, which additionally promotes the formation of the uncracked ligament. This formulation is a future work. It is further noted that the present model has a cell-size dependency. To reproduce a crack arrest length agreeing with experiment, the value of $a_w$ was determined by comparing the calculation and experiment. Simulation including accurate arrest crack length is a future work.

Recent heavy-section high crack-arrest toughness steel plates exhibit fracture surface morphologies which are different from those of the conventional steel plates$^{1,2}$. Crystallographic anisotropy, as well as toughness distribution in the thickness direction might be a reason to this. The present model is expected to apply to these steels in the future study.

### 6. Conclusions

A numerical simulation model of crack propagation was developed and it was validated by small-scale crack arrest test of steel. And mechanisms of the formation of fracture surface irregularities was discussed. Main conclusions derived from the present study are as follows:

1. Chevron markings are not a consequence of the merging of a propagating main-crack and a crack independently initiated ahead of the main crack but they are a nucleation and continuation of ridges formed between two cleavage crack terraces having different height levels.

2. Extent of the chevron markings, or depth of a ridge, changes along with a change of stress intensity factor even at the same test temperature. This result is understood from the present numerical model, i.e., a deep ridge reduces local stress intensity factor through shear stress acting on the ridge and the deep ridge can develop only at high stress intensity level but only shallow ridges are possible if stress intensity level is low. This tendency agreed between the experiment and the numerical simulation.

3. The present numerical simulation model indicates that a crack front near the mid-thickness of a plate tends to precede that near plate surfaces, exhibiting crack tunneling but a propagating crack front shape is not always the same with an arrested crack
front shape. The tunneling becomes pronounced just before crack arrest because a cleavage crack is arrested near the plate surfaces, and active (propagating) crack front becomes limited near the mid-thickness of the plate. In other words, the crack arrest is not sudden but gradual. Direction of a chevron marking lines does not always have a right angle with propagating crack front.

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