Micromechanical Modeling of Ductile Crack Initiation Behavior of Two Phase Steels

Nobuyuki ISHIKAWA, David M. PARKS1) and Masayoshi KURIHARA2)

Formerly Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue Cambridge, MA 02139 USA. (Visiting Scientist from NKK Corporation) Now at Materials and Processing Research Center, NKK Corporation, Kokan-cho, Fukuyama 721-8510 Japan. 1) Department of Mechanical Engineering, Massachusetts Institute of Technology, 77 Massachusetts Avenue Cambridge, MA 02139, USA. 2) Materials and Processing Research Center, NKK Corporation Minamiwatarida-cho, Kawasaki-ku, Kawasaki, 210-0855 Japan.

(Received on August 21, 2000; accepted in final form on October 17, 2000)

The effects of the volume fraction and the morphology of a second phase on ductile crack initiation behavior were determined by notched round bar tensile specimens using ferrite–pearlite steels which contain quite small amounts of MnS inclusions. Nominal strain to crack initiation was increased by decreasing pearlite volume fraction, and by the controlled rolling, which produces an elongated microstructure. The Gurson–Tvergaard (G-T) constitutive model was used to investigate the micromechanism of ductile crack initiation behavior. For evaluating the void nucleation strain, an axisymmetric unit cell model based on a Voronoi tessellation of the BCC lattice (V-BCC model) was applied to determine the microscopic strain inside the pearlite phase which controls secondary void nucleation. The parameter representing the volume fraction of nucleated void, \( f_v \), was evaluated by fitting the numerical solution to experimental data for nominal stress/nominal strain curves of the notched round bar specimen. It was found that steels with lower pearlite volume fractions or elongated pearlite nodules have lower \( f_v \) and the void growth rate is lower for the steels with lower \( f_v \) which requires a large amount of plastic strain for void growth. Ductile cracking was initiated in the region having the highest void volume fraction for all steels. It was shown that the critical void volume fraction for ductile crack initiation is independent of stress triaxiality, and the steels with lower \( f_v \) show smaller critical void volume fractions.

KEY WORDS: structural steel; ferrite–pearlite steel; ductile fracture; void nucleation; void growth; crack initiation; FEM analysis; unit cell model.

1. Introduction

In many steels, the process of ductile fracture is explained by the growth and coalescence of voids which initiated at inclusions such as oxides or sulfides. Void growth is accelerated by a triaxial stress state,\(^1,4\) and many investigations have been done on ductile crack initiation criterion in relation to the void growth rate.\(^3,4\) Recently the Gurson–Tvergaard (G-T) constitutive model was used for void-containing materials, which was originally proposed by Gurson\(^5\) and later modified by Tvergaard,\(^6,7\) has been widely used for the investigation of ductile fracture.\(^8–12\) The G-T model can demonstrate softening behavior of a material in relation to void growth, and an empirical criterion for void coalescence has been associated with a critical void volume fraction.\(^13\) In this model, the initial void volume fraction is typically taken to be the same as the volume fraction of nonmetallic inclusions.\(^13–15\) Void growth from MnS inclusions plays a dominant role on ductile crack initiation in regions with a high triaxial stress state, such as a crack tip region and the center region of a fully-plastic notched specimen.\(^4\) However, as refining techniques in the steel making process have been improved, recent commercially-produced structural steels contain much fewer inclusions.\(^16\) Ishikawa et al.\(^17\) showed that the ductile crack initiation in ferrite–pearlite steels with very small amounts of MnS inclusions, and ductile crack initiation in regions of strain concentration, but with a low stress triaxiality, are both controlled by secondary void nucleation from pearlite nodules. It was also pointed out that the parameters in the G-T model should be closely related with the details of the microscopic behavior of materials.

In order to improve the ductility of steels, it is important to understand the mechanism of ductile crack initiation behavior. However, the void nucleation and growth mechanism is not yet sufficiently clear, even in ferrite–pearlite steels. For this reason, many parameters in the G-T model need to be determined by parameter fitting with experimental data or certain parameters are set at particular values without fully considering the physical meanings for those parameters.

In this study, notched round bar tensile tests were conducted using ferrite–pearlite two-phase steels differing in microstructural characteristics such as pearlite volume frac-
tion, shape and distribution of pearlite particles, and the effects of such microstructural characteristics on notched ductility were investigated. The G-T constitutive model was applied to evaluate stress/strain state and void volume fraction in the critical regions where ductile cracking occurs. The void nucleation parameters in the G-T model are closely related to microstructural characteristics of the ferrite and pearlite phases. The void nucleation strain, one of the major parameters in the G-T model, was determined in relation to the microscopic behavior of the pearlite phase. In order to simulate the microscopic behavior of two-phase steels with different microstructures, finite element unit cell models based on a Voronoi tessellation of the BCC lattice were used. The critical void volume fraction for ductile crack initiation was investigated, and the effect of morphological characteristics on void nucleation and growth behavior was also discussed.

2. Ductile Crack Initiation Behavior of Notched Round Bar Specimens with Different Pearlite Morphologies

2.1. Materials and Experimental Procedures

In order to investigate the effect of pearlite volume fraction on ductile crack initiation behavior, three types of steels with different carbon contents were tested. Chemical compositions and mechanical properties of the steels are shown in Table 1. The carbon content varies from 0.033 to 0.153 mass%. Addition of microalloying elements, such as Nb and V, was increased for lower carbon steels in order to obtain the same level of tensile strength as that of the higher carbon steels. Steel plates with a thickness of 25 mm were produced mainly by conventional rolling processes, while controlled rolling was also applied to the 0.153% C and 0.033% C steels in order to obtain different pearlite morphologies. However, all steel plates were air cooled after finishing rolling in the austenite temperature range. Figure 1 shows microphotographs of the steels. All steels have ferrite–pearlite microstructure, but the volume fraction and the morphology of pearlite vary, depending on the carbon content and the rolling process. It is obvious from Fig. 1 that ferrite grain size decreases under controlled rolling conditions, and the microstructure is quite elongated along the rolling direction, especially for Steel D2.

Morphologies of the two-phase steels can be characterized by the following geometrical parameters: the volume fraction of the second phase, \( \rho_{\text{pearlite}} \); the particle aspect ratio, \( R_a \); and the neighboring factor, \( N_f \). A schematic idealization of the microstructure, used to illustrate the morphological parameters, is shown in Fig. 2. The aspect ratio is given by \( R_a = \frac{b}{a} \), where \( b \) and \( a \) are the average nodule sizes in the rolling direction and in the transverse direction, respectively. The neighboring factor is defined as,

\[
N_f = \frac{\lambda_L}{\lambda_T}, \quad (1)
\]

where \( \lambda_L \) and \( \lambda_T \) are the average center-to-center spacings of the pearlite nodules in the rolling direction and in the transverse direction, respectively.

| Steel | Chemical composition (mass. %) | Manufacturing process | YS (MPa) | TS (MPa) | EL (%) | RA (%) |
|-------|--------------------------------|-----------------------|----------|----------|--------|--------|
| D1    | 0.153 0.39 1.35 0.016 0.004 0.010 | Conv. | 337 529 | 38 77 |
| D2    | 0.085 0.33 1.34 0.015 0.003 0.028 | CR | 412 536 | 39 79 |
| E1    | 0.035 0.31 1.14 0.016 0.001 0.034 0.040 CuNi | Conv. | 366 495 | 39 78 |
| F1    | 0.035 0.31 1.14 0.016 0.001 0.034 0.040 | Conv. | 390 495 | 37 80 |
| F2    | 0.035 0.31 1.14 0.016 0.001 0.034 0.040 | CR | 391 464 | 43 84 |

* Conv.: Conventional rolling, CR: Controlled rolling

Fig. 1.

Microphotographs of the ferrite–pearlite steels.
The pearlite volume fraction was measured with an image analyzer, averaging over about 10 different photographs. The MnS volume fraction, the aspect ratio and the neighboring factor were also measured using the same photographs, and the obtained values are listed in Table 2. The MnS volume fractions are quite small for all steels because of very low sulfur contents. The pearlite volume fraction varies from 1.2% to 18.8%, depending on the carbon content and the rolling process. Comparison of Steels D1 and D2 shows that the aspect ratio and the neighboring factor are obviously increased by the controlled rolling. On the other hand, there is not a large difference in the pearlite morphology between Steel F1 and Steel F2, although pearlite volume fraction is smaller for Steel F2. Ferrite grain sizes are also listed in Table 2.

Ductile crack initiation behavior was examined by using notched round bar specimens, as shown in Fig. 3. The specimens were machined from the steel plates along the rolling direction. All specimens have a gauge length of 26 mm and a notch depth of 2 mm. Three types of the specimens with different root radius were used for the test to obtain different triaxial stress states around the notch region. Tensile tests were conducted under a quasi-static loading rate, and displacement across the gauge length was measured with a clip gauge attached to the specimen.

2.2. Effect of Pearlite Morphology on Ductile Crack Initiation Behavior

Nominal stress/nominal strain curves of notched round bar specimens for Steel E1 with different notch root radius are shown in Fig. 4. Maximum nominal stress decreases and nominal strain to failure increases with increasing root radii. Several specimens with the same root radius were used, and loading tests were interrupted at different displacements before breaking of the specimens. Crack initiation points were determined by microscopic observation of the notch region in the center section parallel to the loading direction. Fig. 5 shows the relation between nominal strain to crack initiation and root radius. Nominal strain to crack initiation increased with increasing root radius for all steels. Ductile cracking occurred in the center of the specimen with \( ρ = 1.0 \text{ mm} \) for all steels. In the specimens with sharper notches, ductile crack initiation was observed in the notch root for all steels excepting Steel F2, in which ductile cracking was initiated in the center for the specimen with \( ρ = 0.25 \text{ mm} \). Thus, the present data indicated that decreasing the pearlite volume fraction and applying the controlled rolling both improve resistance to ductile crack initiation.

3. Micromechanical Modeling of Void Nucleation and Growth Behavior

3.1. The Gurson–Tvergaard (G-T) Constitutive Model

The G-T model assumes plastic flow of a void-containing material as a continuum, and the effect of the voids is averaged through the material. A yield condition for the void-containing material is written as
and Steninger 23) observed void nucleation at pearlite nodules as a result of cracking in the pearlite colony. Qiu et al. 24) also observed that pearlite nodules are a major nucleation site for the secondary voids, and nucleation of the secondary voids depends strongly on applied plastic strain. It is considered that when the crack propagates across the entire pearlite nodule during plastic deformation, the crack behaves as a void, as shown in Fig. 6, and the void nucleation strain is defined as the macroscopic strain at this stage. Subsequently, the nucleated void grows in accordance with the void growth theory given by Eq. (4). Qiu et al. 24) suggested the void nucleation strain as \( \varepsilon_{\text{eq}} = 0.36 \) for a ferrite–pearlite steel with similar pearlite volume fraction and tensile properties as Steel D1.

The standard deviation, \( s_N \), which is mainly based on inhomogeneity of shape or distribution of void nucleation sites, was chosen as \( s_N = 0.1 \) in this study same as many investigations on structural steels. 8,9,10,17,21)

The volume fraction of nucleated void, \( f_N \), is closely related to microstructural characteristics of the ferrite–pearlite steels. 17) If all of the pearlite nodules in the critical region crack and act as secondary nucleated voids, the volume fraction of the nucleated voids, \( f_N \), is given by

\[
f_N = V_{\text{void}}/V_{\text{pearlite}}
\]

where \( V_{\text{void}} \) and \( V_{\text{pearlite}} \) are the volume of the nucleated void caused by cracking of a pearlite nodule, the volume of the pearlite nodule, as indicated in Fig. 6, and the pearlite volume fraction of the steel, respectively. However, it is difficult to experimentally obtain the exact values of the void volume nucleated per pearlite nodule, \( V_{\text{void}}/V_{\text{pearlite}} \) for each steel. Therefore, \( f_N \) was determined by fitting of numerically obtained nominal stress/nominal strain curves using G-T model and experimental data, which will be discussed later.

4. Investigation of the Void Nucleation Strain Using Finite Element Unit Cell Model

4.1. Voronoi Tessellation of the BCC Lattice (V-BCC) Model

Socrate and Boyce 18) proposed an axisymmetric finite element unit cell model to investigate the macroscopic and microscopic stress–strain behavior of toughened polycarbonate. This axisymmetric unit cell model (V-BCC model) is based on a Voronoi tessellation of the BCC lattice, which, when compared with traditional straight-side axisymmetric cylindrical unit cells, better represents the spatial distribution of voids or second-phase particles.

In order to determine stress/stress conditions in the pearlite phase, the V-BCC model was used in this study. In this model, the truncated octahedron as the Voronoi cell of the BCC lattice is used for a space-filling polyhedron as shown in Fig. 7(a). The second-phase particles are arranged on a regular BCC lattice. Because of the periodic symme-
try, only half of this Voronoi cell is used for analysis, and this can be treated as axisymmetric unit cell which contains the second-phase particle. Figure 7(b) shows two adjacent axisymmetric Voronoi cells. The initial height of the unit cell was chosen as \( H_0 = 1.0 \). By translating the truncated Voronoi cell into an axisymmetric cell, the initial radius of the cell mid plane \( (z/H_0)^{0.5} \) is given as \( R_0(0.5)/H_0 \). Geometric compatibility of the deformation in the two axisymmetric cells requires the constraint of the radial and axial displacement of the points on the outer boundaries as follows:

\[
(R_0(x) + U_r(x) + U_z(1-x))^2 = 2(R_0|0.5 + U_r|0.5)^2, \quad (9)
\]

where \( U_r(x) \) and \( U_z(x) \) are the radial and axial displacement for a point on the outer boundary of the cell which is at \( z = x \) in the undeformed configuration. \( U_r|0.5 \) and \( U_z|0.5 \) are the radial and axial displacement of the point at the outer radius with initial coordinate of \( (r=R_0|0.5, z=0.5) \), as illustrated in Fig. 7(c).

Equations (9) and (10) define the constraint condition for the outer boundary which must be imposed on the V-BCC cell to account for the antisymmetric adjacent cells which form the BCC lattice. Other boundary conditions are (i) points on the \( z \)-axis and points on the \( r \)-axis are constrained in the radial and axial direction, respectively, and (ii) points on the top plane \( (z=1.0) \) are required to have equal axial displacement.

4.2. FE Models for the Two-phase Steels

FE analyses were carried out to investigate the microscopic response of the ferrite–pearlite steels and the effects of pearlite morphology under monotonic tensile loading. The FE program ABAQUS ver. 5.8 (Hibbitt, Karlsson and Sorensen, Inc.) was used for this analysis. The V-BCC cells were modeled using axisymmetric second-order elements. Figure 8 shows examples of the finite element meshes for two-phase materials used in this analyses. Configurations of these meshes were defined in accordance with the actual microstructure of the ferrite–pearlite steels in which the shape and distribution of the pearlite phase is parameterized by the volume fraction, \( f_p \), the aspect ratio, \( R_a \), and the neighboring factor, \( N_f \). The pearlite particle was modeled as a cylinder capped with a hemispherical end. The Poisson's ratio was taken as 0.3 and the Young's modulus as 206 000 MPa. The Mises criterion for yielding was applied here because the V-BCC model was used to simulate the mechanical behavior of the pearlite phase up to cracking of the pearlite, which leads to secondary void nucleation, and void growth needs not to be considered. The most distinctive characteristics of the V-BCC model are the boundary conditions expressed by Eqs. (9) and (10), and these non-linear displacement boundary conditions were imposed via a “Multi Point Constraint (MPC)” user subroutine in the ABAQUS program.

4.3. Estimation of Stress/Strain Curves for Each Constituent Phase

The definition of a stress/strain relation for each constituent phase is essential for development of micromechanical models to investigate the microscopic behavior of two-phase materials. The stress/strain curve of the pearlite phase in the present ferrite–pearlite steel was experimentally obtained using a fully-pearlitic steel with eutectoid composition of 0.68%C–0.24%Si–0.87%Mn (in mass%) produced by a conventional rolling process maintaining the same cooling rate imposed for the ferrite–pearlite steels.
The ferrite tensile properties, phase steels.

This shows the capability of the V-BCC model in precisely estimating the deformation behavior of the present two-phase steels. Results show good agreement with the experimental data. All calculated stress/strain relations for ferrite phases which were described above.

In order to estimate the stress/strain relation of the ferrite phase, a simplified method to estimate the stress/strain curve for the ferrite phases which exhibits Luders elongation was proposed by Ishikawa et al. by using empirical equations to obtain tensile parameters. In this model, the plastic part of the stress/strain curve, which has a Luders elongation, is expressed as:

$$\sigma = \sigma_0 (1 + \varepsilon) \quad \text{if} \quad \varepsilon \leq \varepsilon_k \quad \text{.........(11)}$$

$$\sigma = F \varepsilon^n \quad \text{if} \quad \varepsilon > \varepsilon_k \quad \text{.........(12)}$$

where $\sigma$, $\sigma_0$, $\varepsilon$, $\varepsilon_k$, and $n$ are the true stress, the true yield strength, which is identical to yield strength $Y_S$, the true strain and the strain at the onset of hardening, respectively. $F$ is called the strength coefficient, and is given by:

$$F = Y_S (1 + \varepsilon_k^n / \varepsilon_k^n) \quad \text{.............(13)}$$

The mechanical properties of pearlite phases in all steels used in this study are almost the same, and the criteria for cracking in the pearlite phases are also taken to be identical for all steels. Figure 10 shows the microscopic plastic strain in the pearlite phase as a function of macroscopic strain of the unit cell calculated by the V-BCC model. The microscopic plastic strain in the pearlite phase was defined as the equivalent plastic strain averaged over the center area of the pearlite phase perpendicular to the loading direction, as illustrated in Fig. 10. The microscopic plastic strain in the pearlite phase increases with the macroscopic strain, but the microscopic strain depends on the steels differing in pearlite content and morphology. When the void nucleation strain of Steel D1 is chosen as $\varepsilon_{WN}=0.36$ according to the experimental data from Qui et al., the corresponding microscopic plastic strain in the pearlite phase is given as 0.172. Assuming that all pearlite phases in the steels used here have the same strain-based local criterion for cracking, the void nucleation strain for the steels other than Steel D1 can be deduced from Fig. 10. The void nucleation strain is obtained as the calculated macroscopic strain of the cell at which the microscopic plastic strain in the pearlite phase reaches a critical value of 0.172. The microscopic plastic strain of Steel D2, which has a highly elongated pearlite morphology, increases more rapidly with the macroscopic strain than does Steel D1, and the inferred void nucleation strain for Steel D2 becomes about half of that of Steel D1. Steels with lower pearlite

![Fig. 9. Comparison of the S-S curves for two phase steels.](Image)

![Fig. 10. Microscopic equivalent plastic strain in the pearlite phase, $\varepsilon_p$, averaged across the center section perpendicular to the loading direction as a function of macroscopic applied strain, $\varepsilon_m$.](Image)

### Table 3. Tensile properties used for the ferrite and pearlite phases.

| Steel | YS (MPa) | TS (MPa) | $\varepsilon_k$ (%) | pearlite phase | YS (MPa) | TS (MPa) | $\varepsilon_k$ (%) |
|-------|----------|----------|---------------------|----------------|----------|----------|---------------------|
| D1    | 347      | 498      | 0.20                | 1.3            | 490      | 837      | 0.26                |
| D2    | 407      | 468      | 0.17                | 2.6            |          |          |                     |
| E1    | 383      | 481      | 0.17                | 1.6            |          |          |                     |
| F1    | 389      | 501      | 0.13                | 0.7            |          |          |                     |
| F2    | 391      | 475      | 0.17                | 2.2            |          |          |                     |

4.4. Analysis of the Void Nucleation Strain

Pearlite itself has a lamellar structure of ferrite and cementite layers, and cracking behavior of the pearlite node depends on lamellar spacing. Porter et al. suggested that cracking of pearlite is caused by shear localization in ferrite layers and subsequent cracking of cementite layers for steels with a relatively large lamellar spacing of about 1 $\mu$m, while necking and fragmentation of the cementite layers is the main cause of nucleation for fine pearlite with lamellar spacing of about 0.1 $\mu$m. In either case, significant plastic strain is needed for cracking in the pearlite nodule, and the void nucleation strain, $\varepsilon_{WN}$, has a close relation with the strain inside the pearlite nodules.

The tensile properties of all the ferrite–pearlite steels used in this study can be assumed to be the same as that of the fully-pearlite steel because the pearlite lamellar spacings are considered to be similar for all the steels. The tensile properties of this fully-pearlite steel are shown in Table 3.

The pearlite lamellar spacings are considered to be similar for the steels used in this study can be assumed to be the same as that of the fully-pearlite steel. The tensile properties of the pearlite phases of all the ferrite–pearlite steels used in this study can be assumed to be the same as that of the fully-pearlite steel because the pearlite lamellar spacings are considered to be similar for all the steels. The tensile properties of this fully-pearlite steel are shown in Table 3.
volume fraction have higher void nucleation strains, while Steel F2 has almost the same void nucleation strain as that of Steel E1. These data for void nucleation strain are listed in Table 4, and are used as void nucleation parameters in the G-T model.

5. FE Analysis of Ductile Crack Initiation Behavior of the Notched Round Bar Specimens

5.1. FE Models Considering the Characteristic Length for Ductile Crack Initiation

FE analysis of the notched round bar specimen was carried out to investigate stress/strain state and void volume fraction around the notch region. The Gurson–Tvergaard constitutive model was implemented into the FE program ABAQUS ver. 5.8 (Hibbitt, Karlsson and Sorensen, Inc.). Axisymmetric second-order elements were used in this analysis. The Poisson’s ratio was taken as 0.3 and the Young’s modulus as 206,000 MPa. True stress/logarithmic plastic strain relation for each steel obtained by smooth round bar tensile test was used as the material data characterizing fully-dense matrix. These stress/strain data were extrapolated by a power law equation to the high strain region after necking of the specimen.

It should be noted that we estimated stress/strain behavior of the ferrite–pearlite steels by the V-BCC models using stress/strain relations for each phase in order to obtain the void nucleation strain in the G-T model. However, we use experimentally-obtained stress/strain curves of the ferrite–pearlite steels in this section in order to precisely simulate tensile behavior of the notched round bar specimens.

For determination of the local stress/strain state or the void volume fraction by FE analysis, we should be careful about the element size where ductile cracking occurs because calculated data are dependent on the element size. Batisse et al. 20 proposed the characteristic length to be the same as the mean spacing of MnS inclusions, and used a finite element having the same size as this characteristic length for FE analysis on a cracked specimen. However, ductile cracking in relatively clean ferrite–pearlite steels is dominated by secondary void nucleation from pearlite nodules. 17 Therefore, a characteristic length for ductile cracking is related to the mean spacing of pearlite nodules, as illustrated in Fig. 11. Examples of the mesh divisions for FE analysis are shown in Fig. 12. It is considered that an area larger than the mean spacing of pearlite nodules is needed to form a macroscopic crack, as shown in Fig. 11. Therefore, the element size in the center of the specimen used here is three times the mean spacing of pearlite nodules indicated in Table 2, both in the lateral and transverse directions. The element size in the notch tip region was chosen as two times the mean spacing of the pearlite nodules, both in the lateral and transverse directions. Only the specimen with \( \rho = 0.1 \) mm for Steel F1 was not able to modeled because the element size in the notch tip region becomes larger than the root radius.

5.2. Evaluation of the Void Nucleation Parameter \( f_N \)

The volume fraction of nucleated void, \( f_N \), was determined by fitting of calculated nominal stress/nominal strain curves using G-T model and experimental data. Figure 13 shows nominal stress/nominal strain curves of the specimen with the root radius of \( \rho = 1.0 \) mm for Steel D1. Nominal stress after the maximum load decreases strongly with increasing values of \( f_N \) and \( f_N = 0.012 \) gives the best fit to the experimental result. Similar analyses were carried out to
determine the $f_N$ value for the other steels from specimens with $\rho=1.0$ mm. The obtained values are listed in Table 4, together with other parameters for the Gurson–Tvergaard model. Steels with smaller pearlite volume fraction have lower values of $f_N$. However, Steel D2, which has almost the same large pearlite volume fraction as Steel D1, also has a low $f_N$ value.

As suggested in Eq. (8), steels with lower $f_{pearlite}$ have lower value of $f_N$ under the same level of $V_{void}/V_{pearlite}$. In comparing Steels D1 and D2, it is considered that $V_{void}/V_{pearlite}$ is smaller for the elongated pearlite (Steel D2) if the opening separation of the crack which occurs in the pearlite nodule is the same, and this may be the reason for the low $f_N$ value for Steel D2.

Using these parameters, FE analysis was conducted on specimens with different root radii. Figure 14 shows nominal stress/nominal strain curves for Steels D1 and F2. All calculated results show good agreement with the experimental curves up to the crack initiation point. After ductile crack initiation, the calculated nominal stress is higher than the experimental one because the finite elements in the critical region were assumed to retain load-carrying capacity even if the void volume fraction exceeds the critical value for ductile crack initiation.

5.3. Local Stress/Strain Conditions for Ductile Crack Initiation

Close examination was carried out on the stress/strain condition in the critical regions where ductile cracking occurs. Figure 15 shows the relation between equivalent plastic strain and stress triaxiality, the ratio of hydrostatic stress to equivalent stress, in the critical region at experimentally-observed point of ductile cracking initiation. The calculated values were taken from the element centroids of the critical regions. The notch tip regions have a lower stress triaxiality of about 0.5, while the centers of the specimens have a higher triaxial stress state. While crack initiation strain decreases with increasing value of the stress triaxiality, as have widely been reported, the sensitivity to stress triaxiality strongly depends on the steels. Steels with lower pearlite volume fraction and steels to which controlled rolling has been applied show higher crack initiation strains, and a significant effect is seen in the low-triaxiality notch tip region. These kinds of differences in the stress/strain states can affect the void nucleation and growth behavior of steels. Void growth behavior up to ductile crack initiation was determined in the next section in order to clarify the dominant parameters for the void growth.

5.4. Evolution of the Void Volume Fraction

Figure 16 shows the radial distribution of void volume fraction in the notch section for Steels D1 and F2, taken from the element centroids (undeformed coordinates).

Fig. 14. Comparison of experimental nominal stress/nominal strain curves and calculated ones.

Fig. 15. Relation between equivalent plastic strain and stress triaxiality in the ductile cracking regions at ductile crack initiation.

Fig. 16. Radial distribution of void volume fraction in the notch section for Steels D1 and F2, taken from the element centroids (undeformed coordinates).
center region has a highest value for both specimens of Steel F2. As indicated in Fig. 5, ductile cracking occurs in the center region for the specimen with \( p = 0.25 \) mm and in the notch tip for the specimen with \( p = 1.0 \) mm; but, the resulting void volume fractions are quite different between Steels D1 and F2. All steels have different void nucleation parameters, as listed in Table 3, and overall void nucleation and growth behavior is strongly controlled by these parameters. Figure 17 shows the evolution of void volume fraction in the critical regions for specimens with \( p = 0.25 \) mm, as a function of the equivalent plastic strain. Void growth behavior depends strongly on the steels, and steels with higher values of \( f_{N} \) generally show higher void growth rates in their notch tip regions. Since the MnS volume fraction is quite small for all steels, and stress triaxiality in the notch tip regions are almost the same, void volume fraction is mainly controlled by the volume fraction of the secondary-nucleated void, which is parameterized by \( f_{N} \). In the case of Steel F2, the void growth rate in the notch tip region is very low, and it can sustain a large plastic deformation at the notch. In turn, this creates substantial plastic strain even in the center region, which also develops a higher triaxial stress state. This causes secondary-void nucleation in the center of the specimen, followed by rapid growth of the voids due to a high triaxial stress, resulting in ductile crack initiation in the center. On the other hand, the plastic strain in the center regions of specimens of the other steels with \( p = 0.25 \) mm does not become large enough, accordingly the void volume fraction in the notch tip region reaches critical conditions before the specimen center does.

Steel D2 shows slightly higher evolved void volume fraction than does Steel E1, even though Steel D2 has a lower value of \( f_{N} \). As listed in Table 4, the characteristics of Steel D2 is its very low value of the void nucleation strain, \( \varepsilon_{N} = 0.19 \), compared to the higher values of \( \varepsilon_{N} = 0.36-0.43 \) for the other steels. This low \( \varepsilon_{N} \) is caused by its highly elongated pearlite shape \( (R_{p} = 2.69) \), which is also the main reason for the small value of \( f_{N} \). Thus, in Fig. 17, the early void nucleation in Steel D2 results in a higher void volume fraction than that in Steel E1 with higher \( f_{N} \).

5.5. Effect of Stress Triaxiality on Critical Void Volume Fraction for Ductile Crack Initiation

The critical void volume fraction, \( f_{c} \), can be defined as the calculated void volume fraction in the critical region at the experimentally-observed ductile crack initiation. Figure 18 shows the critical void volume fraction as a function of the stress triaxiality at the ductile crack initiation. Steels with smaller pearlite volume fractions or steels subjected to controlled rolling, which both tend to have lower values of the volume fraction of nucleated void, \( f_{N} \), show smaller critical void volume fractions, and the critical void volume fraction is independent of stress triaxiality.

There are several reports on the effect of stress triaxiality on the critical void volume fraction. Shi et al.\(^{31}\) experimentally observed void volume fraction around the crack initiation region of notched and fatigue pre-cracked Charpy specimens of structural steels containing 0.008 wt% sulfur, and suggested a strong effect of stress triaxiality the on critical void volume fraction. Zhang and Niemi\(^{32}\) investigated the critical void volume fraction under various triaxial stress states based on the Thomason’s plastic limit-load criterion\(^{31}\) combined with the G-T model for determining void growth behavior, and showed that the critical void volume fraction for materials with relatively large initial void volume fraction, \( f_{p} \), is affected by stress triaxiality, while \( f_{c} \) is almost constant for materials with small values of \( f_{p} \). Ishikawa et al.\(^{17}\) also suggested a constant critical void volume fraction for steels with a small MnS content by comparing experimental investigations and calculation using the G-T model.

The critical condition for ductile crack initiation by void coalescence is considered to be equivalent to a state where the plastic instability of an inter-void matrix takes place.\(^{31}\) It is reasonable that steels with lower \( f_{p} \) have smaller critical void volume fractions, because the void growth rate of the low \( f_{N} \) steel is low, and a large amount of plastic defor-

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Fig. 17. Void volume fraction in the critical region as a function of local equivalent plastic strain for specimens with \( p = 0.25 \) mm. The ends of the curves denote local condition at initiation of ductile cracking, except for the curve for the notch tip of Steel F2.

Fig. 18. Relation between critical void volume fraction and stress triaxiality.
nation is necessary for the void growth. Therefore, reduced hardening and elevated stress levels at large deformation make the matrix material less stable, even at lower levels of void volume fraction.

It should be noted that the calculated void volume fraction is dependent on the element size, as stated before, and use of a different element size gives a different value for the local void volume fraction. There should thus be a strict definition for the element size in order to support wider use of numerical analysis using the same parameters for the G-T model. We chose the element size as three times the mean spacing of the pearlite nodules in the center region of the specimen, and as twice the mean spacing of the pearlite nodules in the notch tip region; either element size contains two inter-void linkages for ductile crack initiation, as illustrated in Fig. 11. Although a precise experimental investigation is expected to clarify the void growth and coalescence behavior, the present definition of the characteristic length is considered to be reasonable, because it is obvious from many experimental investigations \(^{17-24}\) that pearlite nodules are major nucleation sites for the secondary voids.

6. Conclusions

The effects of microstructural characteristics of the ferrite–pearlite steels, such as pearlite volume fraction and its morphology, on ductile crack initiation behavior were determined by the notched round bar tensile test, and the micro-mechanism of ductile crack initiation was investigated based on the Gurson–Tvergaard constitutive model. An axisymmetric unit cell model was applied to evaluate void nucleation for those steels was increased by decreasing the pearlite volume fraction and by controlled rolling, which means that the void nucleation is mainly controlled by the pearlite nodules. Nominal strain to crack initiation for these steels was increased by decreasing the pearlite volume fraction and by controlled rolling, which produces an elongated microstructure.

(2) Secondary void nucleation occurred by cracking of the pearlite nodules, controlled by pearlite plastic deformation, and the local plastic strain inside the pearlite phase was calculated as a function of overall strain by using an axisymmetric unit cell model based on a Voronoi tessellation of the BCC lattice. The void nucleation strain, \(e_{\text{cr}}\), was defined as the macroscopic strain of the cells at which the microscopic plastic strain in the pearlite phase reaches a critical value. Steels with smaller pearlite volume fractions have higher \(e_{\text{cr}}\) while the steels subjected to controlled rolling have lower \(e_{\text{cr}}\).

(3) Notched round bar specimens were modeled using the Gurson–Tvergaard constitutive model, and the element size in the critical regions where ductile cracking occurs was chosen depending on the mean spacing of pearlite nodules. The volume fraction of nucleated void, \(f_{\text{nv}}\), was evaluated by fitting of the numerical solution and experimental data of the notched round bar specimen of largest root radius. Steels with lower pearlite volume fraction or elongated pearlite nodules have lower \(f_{\text{nv}}\).

(4) Ductile cracking was initiated in the region having the highest computed void volume fraction for all steels. Void growth rate was mainly controlled by \(f_{\text{cr}}\) for these clean steels, and the steels with low \(f_{\text{cr}}\) need a large amount of plastic strain for void growth.

(5) The critical void volume fraction for ductile crack initiation is dependent on stress triaxiality, and the steels with lower \(f_{\text{cr}}\) show smaller values of critical void volume fraction at initiation of ductile cracking.

Acknowledgments

The first author would like to thank Prof. M. Toyoda of Osaka University for his beneficial advice. D.M.P. acknowledges partial support from the U.S. D.O.E. under grant number DE-FG02-85ER1331 to MIT.

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