Numerical Simulation of Microstructurally-Short-Crack Propagation in Creep*

Ryuichi OHTANI** and Takayuki KITAMURA**

A stochastic model and a method of numerical simulation of the propagation of a microstructurally-short crack along grain boundaries in monotonic creep were proposed. In the model, a distribution of crack propagation rate at each grain boundary was expressed by means of random variables representing grain boundary length and crack propagation rates at and between two adjacent grain boundary triple points. The cumulative probability of crack length was calculated using a Monte Carlo method to clarify the effect of some factors such as the grain boundary length, the initial crack length, the upper and the lower bounds of crack propagation rates, and the waveform of the crack propagation rate between two adjacent triple points. The lower bound of the crack propagation rate and the initial crack length affected strongly the cumulative probability. The probability of the length of randomly distributed cracks for continuous crack initiation during creep was also simulated on the basis of the model, and it was confirmed to coincide with the experimental results.

Key Words : Creep, Crack Propagation, Short Crack, Stochastic Model, Numerical Simulation, Grain Boundary Triple Point

1. Introduction

In recent years, attention has been paid to the behavior of short-crack propagation of room-temperature as well as high-temperature fatigue and monotonic creep in steels and alloys^{(1)~(7)}. The application of K- or J-based fracture mechanics established for long cracks, however, is questionable in the case of short cracks. In particular, microcracks of less than a few grains in length, which are called microstructurally-short cracks⁽²⁾, show irregular propagation in their path and direction as well as in their rate due to microstructural inhomogeneity. A stochastic approach has been made to explain a scatter of the resistance of long-crack propagation^{(8)~(11)}. A similar concept and methodology cannot be adopted for microstructurally-short-crack propagation, because any definite expression of fracture mechanics laws is insignificant. It is, therefore, necessary to construct a

suitable stochastic model of the short-crack propagation and to make its numerical simulation.

In the present study, the distribution of crack propagation rates between two adjacent grain boundary triple points was given as random variables with reference to the experimental results on short creep cracks. Based on the model, which will be referred to as the crack propagation rate distribution model, a Monte Carlo numerical calculation was conducted to discuss some parameters which were given as dominant factors affecting the short-crack propagation rate. The cumulative probability of the length of distributed cracks on the surface of a smooth specimen during creep was also simulated on the basis of this model.

List of symbols

D : grain boundary length (projection on the plane perpendicular to the applied stress axis)

$D1$: mean value of D

$D2$: standard deviation of D

a : crack length

a_0 : initial crack length

a_c : the smallest length of the crack to which the

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** Department of Engineering Science, Kyoto University, Yoshidahon-machi, Sakyo-ku, Kyoto, 606, Japan

(a) Crack propagation curves

long-crack propagation law is applicable
 da/dt : crack propagation rate
 $(da/dt)_U$: upper bound of da/dt along each grain boundary
 $(da/dt)_L$: lower bound of da/dt along each grain boundary
 U : upper confidence limit of da/dt
 DU : median of $(da/dt)_U$
 DL : median of $(da/dt)_L$
 c : coefficient of the $da/dt - a$ relation for a long through-crack
 M : number of cracks calculated (or number of cycles of calculation)
 t_s : crack propagation time calculated
 $F(a)$: cumulative distribution function of crack length for a single crack
 $\Phi(a)$: cumulative distribution function of crack length for distributed multiple cracks in a material

2. Method of Numerical Analysis

2.1 Crack propagation model

Figures 1(a) and (b) show typical propagation curves and propagation rate curves of microstructurally-short creep cracks observed on the surface of a smooth specimen of 304 stainless steel with a grain size of $500 \mu\text{m}^{(12)}$. The creep test was conducted under a stress of 117.7 MPa at a temperature of 973 K (700°C) in a vacuum. The characteristics of the crack propagation behavior are summarized as follows.

(1) The cracks initiated at grain boundary triple points or carbide precipitates propagate at high rates along grain boundaries and decelerate when they hit

(b) Relation between crack propagation rate and crack length

Fig. 1 Experimental results on microstructurally-short-crack propagation in creep at the surface of a smooth specimen of 304 stainless steel

triple points or sharp bends in grain boundaries.

(2) The relation between crack propagation rate and crack length varies greatly with individual cracks. Upper and lower bounds of the fluctuation of

crack propagation rates tend to be out of the scatter band of the $da/dt - a$ relation for long through-cracks.

(3) The fluctuation seems to merge in the scatter band of long cracks as the crack length becomes longer than about the size of one grain.

Similar results were obtained in other experiments on creep and high-temperature low-cycle fatigue of another 304 stainless steel with a grain size of $40 \mu\text{m}$, although the smallest length of cracks to which the long-crack propagation law is applicable was equal to three or five times the grain size^{(7),(13)}.

According to the experimental results, the following model was constructed.

(i) The crack length is the length of projection of a crack on the plane perpendicular to the applied stress axis. The grain boundary length between two adjacent triple points, which is also the length of projection on the plane perpendicular to the stress axis, is given as random variables of a normal distribution.

(ii) The intergranular crack propagates at alternately increasing and decreasing rates between the upper and lower bounds of the rate, as shown in Fig. 2(a). The lower bound appears at a grain boundary triple point.

(iii) The upper and the lower bounds of the propagation rate are given as random variables of logarithmic normal distributions with medians shown by the chain line and the double chain line in Fig. 2(a), and the respective upper confidence limits by the horizontal dashed line and the 45°-inclined solid line in Fig. 2(a). When the crack length is longer than a_c , the scatter in the crack propagation rate becomes small and it follows the relation for long through-cracks given by

$$da/dt = ca \quad (1)$$

which is indicated by the solid line in Fig. 2(a).

(iv) The crack propagation rate between grain boundary triple points is given as it varies in a triangular waveform shown in Fig. 2(b). The rate is expressed by the following equations:

$$da/dt = L_1 \exp(m_1 h) \quad (2)$$

between the points A and B

$$da/dt = L_2 \exp(m_2 h) \quad (3)$$

between the points B and C

where

$$h = (a - a_1)/D \quad (4)$$

and a_1 is the crack length at the point A. L_1 and m_1 are obtained from the values of da/dt at the points A ($h=0$) and B ($h=1/2$), and L_2 and m_2 , at the points B and C ($h=1$).

2.2 Method of numerical simulation

On the basis of this model, numerical calculation of the crack propagation curves was done using ran-

dom numbers, and the results are shown in Fig. 3(a). The input data for the calculation are also listed in Fig. 3(a), which were determined by using the experimental results shown in Fig. 1. The irregular simulation curves are analogous to the actual propagation curves.

Another numerical simulation based on a statistical differential equation,

$$da/dt = Ga \quad (5)$$

was done for comparison. In Eq. (5) G is a probability density function of a logarithmic normal distribu-

	$a \geq a_c$		$a < a_c$	
	Median	Upper confidence limit (U%)	Median	Upper confidence limit (U%)
$(da/dt)_u$	$\ln(\sqrt{2}ca)$	$2ca$	$\ln[\sqrt{2}cae \cdot (a/a_c)^{0.414}]$	$2cae$
$(da/dt)_L$	$\ln(ca/\sqrt{2})$	ca	$\ln[cae(a/a_c)^{2.414}/\sqrt{2}]$	ca

(a) Relation between crack propagation rate and crack length

(b) Crack propagation rate at a grain boundary between two adjacent triple points

Fig. 2 Illustration of the proposed model on micro-structurally-short-crack propagation in creep

tion of the short-crack propagation rates with the median shown by the solid line in Fig. 2(a) or Eq. (1) and the upper confidence limit shown by the horizontal dashed line in Fig. 2(a). Figure 3(b) shows the calculated result, indicating that Eq. (5) cannot represent the irregular propagation curves but gives a rather smooth curve.

The crack length after propagating until the time, t_s , from the initial length, a_0 , is not constant, but shows a distribution, because the crack propagation curves vary greatly with individual cracks. The cumulative distribution can be obtained by means of the Monte Carlo method. In order to determine the number of cycles of calculation, the Monte Carlo simulation was done for M pieces of crack. The result is

(a) Crack propagation curves based on the proposed model

(b) Crack propagation curve based on a statistical differential equation (Eq. (5))

Fig. 3 Results of the numerical simulation of crack propagation curves

shown in Fig. 4. The input values except the value of M were fixed in each calculation and listed in Table 1, which were based on an experimental result^{(13),(14)} of 304 stainless steel with the grain size of $40 \mu\text{m}$ subjected to a stress of 147.1 MPa at a test temperature of 923 K (650°C) in air and ruptured at about 100 h . It is found from Fig. 4 that the distribution curves converge into a unique curve when the value of M is more than about 100 . Therefore, the value $M=300$ was adopted for the present calculation.

3. Results of Calculation and Discussion

In this chapter, calculated results on the cumulative distribution of crack length are shown and comments are made on the effect of some parametric factors on the short-crack propagation. Standard

Table 1. Standard values used for the numerical simulation

t_s	82h	$D = D1 + \alpha D2$ Average(α)=0 Standard deviation(α)=1
$D1$	0.02mm	
$D2$	0.005mm	
α_0	0.01mm	
U	95%	
c	0.0226 h^{-1}	
M	300	
a_c	0.1mm

Fig. 4 Effect of number of cracks (number of calculation) on the cumulative distribution of crack length

values of the factors are shown in Table 1.

3.1 Effect of crack propagation time

Figure 5 illustrates the effect of crack propagation time, t_s , on the cumulative distribution of crack length, $F(a)$. The distribution curves hardly change for $F(a) < 0.5$, while they vary remarkably depending on t_s for $F(a) > 0.8$. This indicates that the early crack propagation has a high probability of being blocked by the first grain boundary triple point, and the crack propagates faster once it passes through the triple point and becomes longer than two grain boundary length. A similar tendency can be found for the multiple surface cracks of smooth specimens.

3.2 Effect of grain boundary length

Figure 6 shows the effect of mean grain boundary length, $D1$, on the cumulative distribution of crack length, $F(a)$. The distribution curves become steep when the crack hits the triple points (at the crack length $a = 0.025$ and 0.075 mm in the case of $D1 = 0.05$

mm), indicating deceleration of the crack propagation by triple points. It is obvious that the distribution curves shift to the right side as $D1$ is large. This suggests that coarse-grained materials have higher crack propagation rates than fine-grained materials. However, the effect of grain boundary length or grain size is not distinguished for rather fine-grained materials, as the curve for $D1 = 0.02$ mm differs little from that for $D1 = 0.05$ mm. On the other hand, it can be interpreted from Fig. 7 that the standard deviation of grain boundary length, $D2$, has little influence on the propagation.

3.3 Effect of initial crack length

Figure 8 shows the effect of initial crack length, a_0 , on the distribution. A large initial crack length brings a high rate of crack propagation. Especially when $2a_0$ is longer than a grain boundary length, $D1$, the distribution curve locates at far longer crack lengths.

Fig. 5 Effect of crack propagation time on the cumulative distribution of crack length

Fig. 7 Effect of standard deviation of grain boundary length on the cumulative distribution of crack length

Fig. 6 Effect of grain boundary length (distance between two adjacent triple points) on the cumulative distribution of crack length

Fig. 8 Effect of initial crack length on the cumulative distribution of crack length

3.4 Effect of upper and lower bounds of crack propagation rates at each grain boundary

Figure 9 shows the effect of upper confidence limit, U , of the upper and lower bounds of crack propagation rates at each grain boundary between two adjacent triple points. It is found that the upper confidence limit hardly affects the cumulative distribution of crack length, except for $F(a) > 0.9$ in the case of the small value of U (or the large standard deviation).

The standard values were used for the values of the medians of logarithmic normal distributions of the upper bound and the lower bound of crack propagation rates in the present calculation, which are shown

Fig. 9 Effect of confidence limits of upper and lower bounds of crack propagation rate on the cumulative distribution of crack length

$(da/dt)_U$

	$a \geq a_c$	$a < a_c$
DU-H		$\ln[\sqrt{2}ca_c(a/a_c)^{0.100}]$
DU-M	$\ln(\sqrt{2}ca)$	$\ln[\sqrt{2}ca_c(a/a_c)^{0.414}]$
DU-L		$\ln[\sqrt{2}ca_c(a/a_c)^{0.666}]$

$(da/dt)_L$

	$a \geq a_c$	$a < a_c$
DL-H		$\ln[ca_c(a/a_c)^{1.487}/\sqrt{2}]$
DL-M	$\ln(ca/\sqrt{2})$	$\ln[ca_c(a/a_c)^{2.414}/\sqrt{2}]$
DL-L		$\ln[ca_c(a/a_c)^{6.027}/\sqrt{2}]$

Fig. 10 Illustration of input data on the medians of upper and lower bounds of crack propagation rates

by the chain line and the double chain line in Fig. 2(a), respectively, and are given by $DU-M$ and $DL-M$ in Fig. 10. In order to examine the effect of the medians on the crack length distribution, two other sets of median values, $DU-H$ and $DU-L$ for $(da/dt)_U$ and $DL-H$ and $DL-L$ for $(da/dt)_L$, as shown in Fig. 10, were chosen for the calculation. The results are shown in Figs. 11 and 12. Figure 11 indicates that the upper bound of crack propagation rate which occurs at the midpoint of a grain boundary has a small influence on the distribution. On the other hand, it can be recognized from Fig. 12 that the lower bound affects the distribution remarkably. These results point out that the deceleration or the temporary arrest of crack propagation at triple points or some obstacles is quite efficient for increasing the resistance of crack propagation.

3.5 Effect of waveforms of crack propagation rate at each grain boundary

In the foregoing results of the calculation, the upper bound of the crack propagation rate at each grain boundary was given at the midpoint of the boundary ($h=0.5$) as shown in Fig. 2(b). In this section, additional calculated results are shown in order to discuss the effect of given waveforms of crack propagation rate. Schematic figures of the waveforms for the calculation are illustrated in Fig. 13(a), where the upper bound arises at the points (1) $h=0.5$, (2) $h=0.1$, (3) $h=0.9$ (triangular waveforms), and between two points (4) $0.1 \leq h \leq 0.9$, (5) $0.1 \leq h \leq 0.5$, (6) $0.3 \leq h \leq 0.7$, (7) $0.5 \leq h \leq 0.9$ (trapezoidal waveforms). In these cases, the grain boundary

Fig. 11 Effect of upper bound of the crack propagation rate at each grain boundary on the cumulative distribution of crack length

Fig. 12 Effect of lower bound of the crack propagation rate at each grain boundary on the cumulative distribution of crack length

(a) Waveforms of crack propagation rate. $R1$: mean value of $(da/dt)_L$

(b) Cumulative distributions of crack length.
 $S1 = -6$: mean value of $(da/dt)_U$, $S2 = R2 = 0.5$: standard deviations of $(da/dt)_U$ and $(da/dt)_L$

(c) Cumulative distributions of crack length.
 $S1 = -6$: mean value of $(da/dt)_U$, $S2 = R2 = 1.0$: standard deviations of $(da/dt)_U$ and $(da/dt)_L$

Fig. 13 Waveforms of crack propagation rate between two adjacent triple points and effect of the waveforms on the cumulative distributions of crack length

Fig. 14 Comparison of cumulative distributions of crack length for continuously initiated multiple cracks calculated on the basis of the model with those of distributed cracks measured on the surface of a smooth specimen of 304 stainless steel

length, D , was assumed to be constant and the upper and lower bounds of the crack propagation rate, $(da/dt)_U$ and $(da/dt)_L$, were given as random variables of a log-normal distribution independent of the crack length, in order to give the same propagation time at each grain boundary irrespective of the rate waveforms. Figures 13(b) and (c) show the dependence of cumulative distribution curves on the rate waveforms, leading us to the conclusion that the overall behavior of crack propagation is not affected greatly by the propagation waveforms at each grain boundary.

4. Comparison Between Calculated Results and Experimental Data

In the present calculation, $F(a)$ is a cumulative probability of crack length for a single short crack initiated at the time zero and propagating until the time t_s . It can be said that $F(a)$ also represents a crack length distribution for multiple cracks which were initiated at the same time in a material. In general, the initiation of cracks in a smooth specimen

under creep loading begins at the early stage of creep and continues up to the rupture⁽¹³⁾. An actual distribution of crack length observed in a specimen at a given time, therefore, is brought about not only by the scatter of the crack propagation rate but also by the randomness of the initiation time. For comparison with the actually observed distribution, it is necessary to calculate a cumulative distribution of crack length for distributed multiple-cracks, taking into consideration the distribution of crack initiation time.

When a number of cracks per unit surface area (or a crack density) at a time t is given as $K(t)$, a number of cracks initiated from the time t to $t+dt$ is

$$dn = \frac{dK(t)}{dt} dt = k(t) dt \quad (6)$$

If a distribution function of crack length at t_s for a single crack initiated at t is expressed by $F(t_s - t, a)$, a distribution function for distributed multiple cracks, $\Phi(a)$, can be obtained by the following equation.

$$\begin{aligned} \Phi(a) &= \int_0^{t_s} F(t_s - t, a) k(t) dt / K(t_s) \\ &= \int_0^{t_s} F(t_s - t, a) k(t) dt / \int_0^{t_s} k(t) dt \end{aligned} \quad (7)$$

Assuming that $K(t)$ is proportional to t and $k(t)$ is constant for a given condition of creep⁽¹³⁾, Eq.(7) becomes

$$\Phi(a) = \frac{1}{t_s} \int_0^{t_s} F(t_s - t, a) dt \quad (8)$$

Solid curves in Fig. 14 show the cumulative distributions in Weibull probability diagrams at the times $t_s = 49$ and 82 h, which were drawn based on Eq. (8) by using the values of parameters in Table 1. The figures also include the actual distributions of short cracks obtained from the creep test of a smooth specimen of 304 stainless steel with grain size of $40 \mu\text{m}$ subjected to the stress of 147.1 MPa at 923 K (650°C) in air⁽¹⁴⁾. As the time to rupture in this test was about 100 h , (a) shows the distribution at the middle of the specimen lifetime and (b) shows it near rupture. The calculated curves in both figures agree well with the experimental data. Similar successful results were obtained for other stress levels.

The model and the simulation method proposed in this study will be useful for predicting the anomalous propagation of microstructurally-short cracks for which the assumption of a continuum macro-fracture mechanics breaks down, not only in monotonic creep conditions but also in time-dependent creep-fatigue conditions.

5. Conclusions

Short creep cracks whose length is less than three to five times the grain size in 304 stainless steels grow in a very irregular manner and violate the assumption of a macroscopic continuum in fracture mechanics

because of microstructural inhomogeneities. A crack propagation rate distribution model was proposed to determine the statistical nature of microstructurally-short-crack propagation in creep. A numerical simulation was conducted based on this model and a Monte Carlo method to analyze the effect of some factors influencing the short-crack propagation. The results obtained are summarized as follows.

(1) As a model of intergranular creep crack, the crack propagation rate was assumed to vary as in a triangular waveform along each grain boundary with a lower bound of the rate decelerated at two adjacent triple points and an upper bound of the rate accelerated at the midpoint.

(2) The effect of the upper bound of crack propagation rate, which was represented as random variables of a log-normal distribution, was not significant on the cumulative distribution of crack length, while the effect of the lower bound of crack propagation rate was conspicuous. The difference in the given waveforms of crack propagation rate along a grain boundary was not greatly influential.

(3) The grain boundary length, which was the distance between two adjacent grain boundary triple points and was represented as random variables of a normal distribution, had little effect on the cumulative distribution of crack length. On the other hand, the initial crack length had obvious effects.

(4) A method to obtain cumulative distributions of crack length for multiple cracks generated successively in a material was proposed and a numerical calculation was done to simulate the experimental data of short-crack distributions on the surface of 304 stainless steel. Good agreement was found between the predicted results and the actual ones.

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