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Quantitative prediction of environmentally assisted cracking based on a theoretical model and computer simulation

T. Satoh [a,b,*], T. Nakazato [b], S. Moriya [c], S. Suzuki [d], T. Shoji [a]

[a] *Division of Fracture Physics and Chemistry, Research Institute for Fracture Technology, Faculty of Engineering, Tohoku University, Aoba-ku, Sendai 980-8579, Japan*

[b] *Scientia, 2-20-13 Teraoka, Izumi-ku, Sendai 981-3204, Japan*

[c] *Rocket High Altitude Performance Section, National Aerospace Laboratory Kakuda Research Centre, Koganezawa, Kimigaya, Kakuda 981-1525, Japan*

[d] *Materials Engineering Group, Power Engineering R&D Centre, Tokyo Electric Power Company, 4-1 Egasaki-cho, Tsurumi-ku, Yokohama 230-0002, Japan*

Abstract

This paper describes a comparison between quantitative prediction of environmentally assisted cracking by theoretical modelling and that by finite element method (FEM) computer simulation in terms of film rupture strain at a crack tip. The crack growth rate was simulated on a 1T-CT (one inch-thick compact tension) specimen, which met American Society for Testing and Materials (ASTM) E813, under the slow strain rate test (SSRT) condition by an FEM simulation code, Finite Element Environmentally Assisted Cracking Simulator (FEEACS) for film rupture strain $\varepsilon_f = 10^{-2}$, 10^{-3}, and 10^{-4}. As the theoretical model includes unknown parameters which cannot be determined theoretically, they were evaluated by chi-square fitting method so that the crack growth rates of the theoretical model fit those of FEM computer simulation. In this method the film rupture strain ε_f and the position r where crack tip strain is defined are evaluated. The calculation was carried out for two cases. One is for irradiation-assisted stress corrosion cracking (IASCC), and the other is without irradiation. Parameters for irradiated material are the yield strength $\sigma_y = 980$ MN/m$^{3/2}$, the slope of the current decay $m = 0.5$, and the strain hardening exponent $n = 3$. In the irradiated case the crack growth rates obtained by the theory agree well with those obtained by FEM using the relation $\varepsilon_{f\ \mathrm{Theory}} = 3.1\varepsilon_{f\ \mathrm{FEM}}$, while they do not agree in the case without irradiation.

1. Introduction

Quantitative prediction of environmentally assisted cracking (EAC) is a one of the critical processes in service life prediction and also structural integrity and safety assessment. It is generally recognized that enhanced crack growth in corrosion fatigue in stress corrosion cracking (SCC) and even in a slow strain rate test (SSRT) can be uniquely explained by a synergistic interaction among materials, environment and stresses for given material/environment systems. The difference in loading modes such as a cyclic load, a monotonically rising load, a constant load and a constant displacement has significant effects on crack tip strain rate which controls both film rupture frequency at a growing crack tip and, subsequently, resultant metal dissolution. Under the neutron-irradiated condition, mechanical properties of materials such as yield strength and strain hardening can be markedly changed, which in turn have significant effects on crack tip strain rate accompanied by other microstructural alternations such as changes in local grain boundary chemistry. Irradiation-assisted stress corrosion cracking (IASCC) is a potential problem in light water reactors (LWRs) when plant life extension is taken into consideration; however, it can be a critical problem in fusion reactors with a water-cooling system.

As has been well recognized, EAC behavior is controlled by so many parameters that it is extremely

* Corresponding author. Fax: +81 22 217 7518.

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difficult to examine the effects of all possible parameters by experiments. Hence, extensive efforts have been focused to develop both EAC models for the various material/environment systems and also quantitative prediction methodology based upon the models. Among the models proposed previously in the literature, the slip dissolution model can provide the most feasible and quantitative prediction for some particular cases providing that the necessary data are available and crack tip strain rate can be adequately evaluated for a given condition.

In this paper, a theoretical prediction of crack growth rates as a function of film rupture frequency is compared with those obtained by a finite element method (FEM) simulation code, finite element environmentally assisted cracking simulator (FEEACS). The theoretical formulation was based upon Faraday's equation for metal dissolution and crack tip strain rate formulation for a growing crack in an elastic/plastic work hardening material under a constant load. The crack tip strain redistribution due to crack advance was taken into consideration in the formulation. The FEM simulation code is based on a slip dissolution model. Both of them did show a mechanics-driven threshold K (stress intensity factor) and a plateau growth rate in the da/dt (crack growth rate)-K diagram. In order to investigate the quantitative relationship between the theoretical model and FEM simulation code, we also compare the crack tip strain rates in both cases. The differences of methodology for lifetime prediction of EAC is discussed quantitatively, and the formulation of the relation between the theoretical method and FEM simulation code in terms of film rupture strain at a crack tip is demonstrated.

2. Procedures

2.1. Theoretical model

Theoretical crack growth rate based upon the slip dissolution model is described as

$$\frac{\mathrm{d}a}{\mathrm{d}t}=\left[\frac{Mi_0t_0^m}{z\rho F(1-m)}\right]\left[\frac{\dot{\varepsilon}_{\mathrm{ct}}}{\varepsilon_{\mathrm{f}}}\right]^m, \tag{1}$$

where M is the atomic weight, ρ the density, z the change in charge due to dissolution, F the Faraday's constant, i_0,t_0 the numerical constants which can be determined by experiments, m the slope of the current decay curve, ε_{f} the rupture strain of protective film at the crack tip, $\dot{\varepsilon}_{\mathrm{ct}}$ the rate of strain at crack tip.

In Eq. (1) the value $\dot{\varepsilon}_{\mathrm{ct}}/\varepsilon_{\mathrm{f}}$ corresponds to film rupture frequency. Plastic strain distribution at a crack tip along the crack line for a growing crack in an elasitc/plastic strain hardening material was developed by Gao et al. [1] as

$$\varepsilon_{\mathrm{p}}=\beta\frac{\sigma_{\mathrm{y}}}{E}\left[\ln\left(\frac{R_{\mathrm{p}}}{r}\right)\right]^{\frac{1}{(n-1)}}, \tag{2}$$

where β is the dimensionless constant, σ_{y} the yield strength, E the elastic modulus, r the distance from a growing crack tip, R_{p} the plastic zone size, n the strain hardening exponent in power law of Ramberg–Osgood stress–strain relations.

When small-scale yielding is assumed, the plastic zone size is given as

$$R_{\mathrm{p}}=\lambda\left[\frac{K}{\sigma_{\mathrm{y}}}\right]^2, \tag{3}$$

where λ is dimensionless constant, K the stress intensity factor.

Consequently, the crack growth rate formula considering the growing crack [2] is described as

$$\frac{\mathrm{d}a}{\mathrm{d}t}=\left[\frac{Mi_0}{z\rho F(1-m)}\right]\left[\frac{t_0}{\varepsilon_{\mathrm{f}}}\right]^m \times\left[\frac{\beta\sigma_{\mathrm{y}}n}{E(n-1)}\left[2\frac{\mathrm{d}K/\mathrm{d}t}{K}+\frac{\mathrm{d}a/\mathrm{d}t}{r}\right] \times\left[\ln\left[\frac{\lambda}{r}\left(\frac{K}{\sigma_{\mathrm{y}}}\right)^2\right]\right]^{1/(n-1)}\right]^m. \tag{4}$$

2.2. Finite element method (FEM)

The computer simulation analysis by FEM was carried out on a 1T-CT specimen under the condition of SSRT with a loading rate of 8.33×10^{-7} mm/s. The specimen geometry and the mesh shape of FEEACS [3] are shown in Fig. 1, where an 8-point isoparametric element was used. This code is based upon a slip dissolution model, and the crack tip strain rate is evaluated by two-dimensional FEM elastic–plastic analysis. The simulation was performed for the film rupture strains $\varepsilon_{\mathrm{f}}=10^{-2}$, 10^{-3}, and 10^{-4} with fixed finest mesh size of 65×65 μm^2 at the crack tip. The crack growth process was simulated by means of a nodal force release technique.

3. Conditions

The common parameters that are used in both methods are listed in Table 1. Table 2 shows the parameters for the irradiated/non-irradiated condition. A yield strength of 100 kgf/mm^2 (980 MN/m^2) was considered as a typical value for austenitic stainless steels after irradiation up to 5×10^{25} neutrons/m^2 ($E>1$ MeV). Non-irradiated yield strength was set to be 20 kgf/mm^2 (196 MN/m^2). As the major dissolved ion was iron, the density and the atomic weight of iron was used

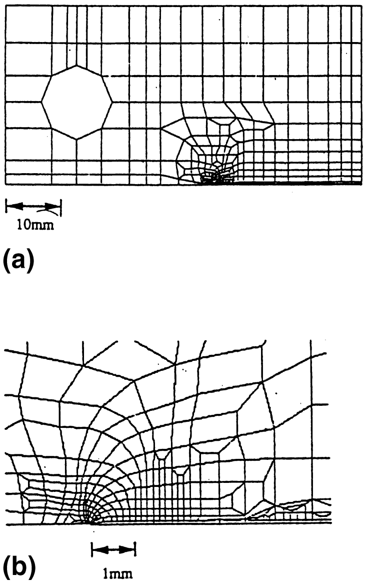

Fig. 1. Finite element mesh for 1T-CT. (a) upper half of the specimen (b) detail around the crack.

for the parameters of the slip dissolution model calculation.

As the theoretical model includes the free parameters which cannot be determined theoretically, they were searched by the chi-square fitting method so that the crack growth rate values of the theoretical model fit those of FEM computer simulation in the d*a*/d*t*–*K* diagram (See Fig. 3). These searched parameters are film rupture strain ε_f and the position *r* where crack tip strain defined.

The value d*K*/d*t* obtained by FEM simulation was substituted into the theoretical formula Eq. (4), as it is a given parameter. Though d*K*/d*t* is a function of *K* in general, it can be considered as a constant in the region of simulation. The value of d*K*/d*t* calculated by FEM simulation and used in the theoretical model are listed in Table 3. Though the position *r* used in the theory should be also given as a function of *K*, the crack growth rate depends little on *r* if the position *r* is far enough from crack tip. Therefore the value *r* was set constant in this work.

Table 2
The parameters irradiated/non-irradiated condition

		Irradiated	Non-irradiated
σ_y	yield strength strain hardening exponent in power law of	980 (MN/m^2)	196 (MN/m^2)
n	Ramberg–Osgood	3	10
m	slope of the current decay curve	0.5	0.8

4. Results and discussion

Fig. 2 shows the relation between the searched film rupture strains $\varepsilon_{f\ \mathrm{Theory}}$ and those used in FEM simulation $\varepsilon_{f\ \mathrm{FEM}}$. In this figure it seems that $\varepsilon_{f\ \mathrm{Theory}}$ agrees well with $\varepsilon_{f\ \mathrm{FEM}}$. Fig. 3 shows the relation between stress intensity factor *K* and crack growth rate d*a*/d*t*. In the irradiated case (a) the crack growth rate d*a*/d*t* obtained by Eq. (3) agreed well with the FEM simulation results. In the case without irradiation (b), however, the tendency of crack growth rates obtained by theory are considerably different from those obtained by FEM in Fig. 3.

In Eq. (1), which was derived from a slip dissolution model, the term $\dot{\varepsilon}_{ct}/\varepsilon_f$ is considered to be a film rupture frequency. As mentioned before, both methods are based on a slip dissolution model, and it has been reported that the relation between crack growth rate and film rupture frequency in FEM satisfies Eq. (1) [4]. Therefore the relation between theory and FEM is described as

$$\frac{\dot{\varepsilon}_{ct\ \mathrm{Theory}}}{\varepsilon_{f\ \mathrm{Theory}}} = \frac{\dot{\varepsilon}_{ct\ \mathrm{FEM}}}{\varepsilon_{f\ \mathrm{FEM}}}. \quad (5)$$

As the error of Gauss–Legendre integral used in this FEM simulation becomes large in the element which includes the crack tip, strain distribution becomes a function of mesh size at the crack tip. On the other hand, in the theoretical model strain distribution is expressed

Table 1
Common parameters used in FEM simulation and in theory

M	atomic weight	5.5847×10^{-2} (kg/mol)
ρ	density	7.86×10^{3} (kg/m^3)
z	change in charge due to dissolution	2.67
F	Faraday's constant	96500 (C/mol)
i_0	initial current density	50 (A/m^2)
t_0	oxidized film reforming time	0.1 (s)
β	dimensionless constant	5.08
λ	dimensionless constant	0.3
E	elastic constant	2.1×10^{10} (kg/m^2)

Table 3
d*K*/d*t* obtained by FEM simulation and used in theoretical model

	$\varepsilon_{f\ FEM} = 10^{-2}$ ■	$\varepsilon_{f\ FEM} = 10^{-3}$ ♦	$\varepsilon_{f\ FEM} = 10^{-4}$ ▲
Irradiated	1.40×10^{-4}	3.50×10^{-4}	6.60×10^{-4}
Non-irradiated	8.03×10^{-4}	1.02×10^{-3}	1.49×10^{-3}

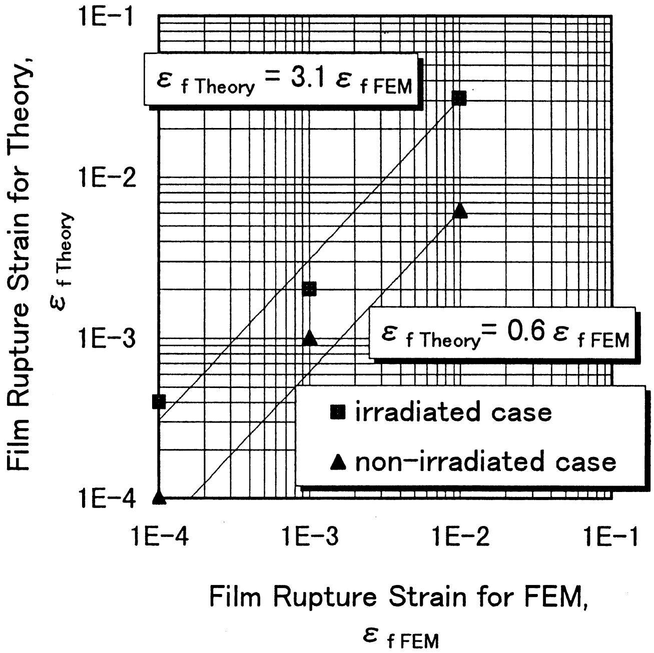

Fig. 2. $\varepsilon_{f\ Theory}$ vs. $\varepsilon_{f\ FEM}$.

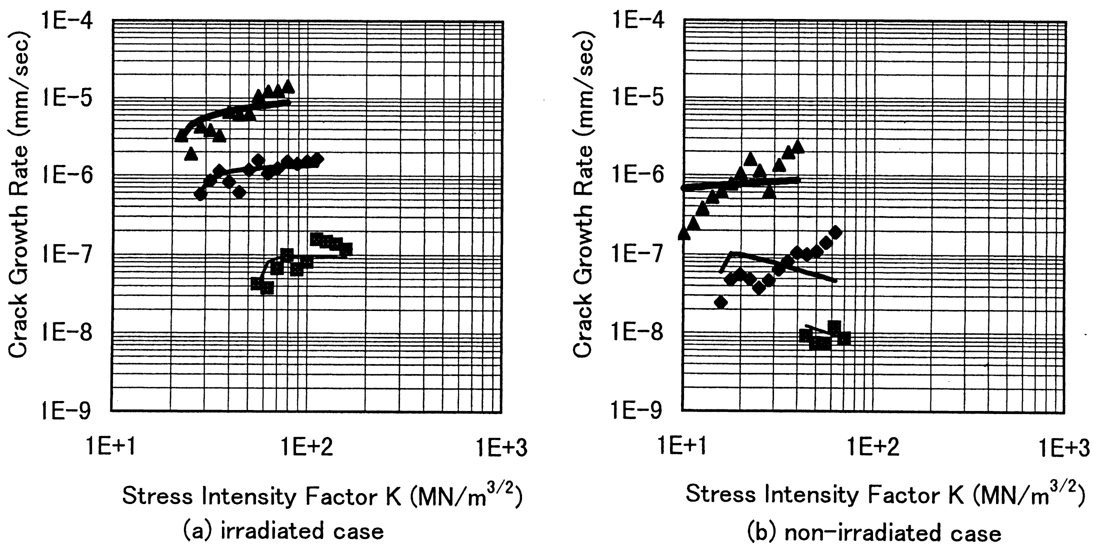

Fig. 3. Crack growth rate vs. stress intensity factor *K*. The dots were obtained by FEM and the lines were obtained from the theoretical model.

by Eq. (2). From Eq. (5), if the constant value C in the relation

$$\varepsilon_{\mathrm{f\ Theory}} = C\varepsilon_{\mathrm{f\ FEM}} \tag{6}$$

is determined, the strain rate in the FEM simulation is expressed as

$$\dot{\varepsilon}_{\mathrm{ct\ FEM}} = (1/C)\dot{\varepsilon}_{\mathrm{ct\ Theory}}. \tag{7}$$

Therefore, in this work the comparison was made in terms of a film rupture strain at crack tip ε_f. In the irradiated case the constant C was 3.1, and in the non-irradiated case it was 0.6. The latter value 0.6 seems to be a suitable result, however, this is not a reasonable value because of the discrepancy in Fig. 1(b). This indicates that the difference between both methods cannot be expressed by adjusting the film rupture strain so as to compensate the FEM mesh size effect. Two causes are taken into consideration. One is that the strain rate for FEM cannot be expressed as Eq. (7). The other is the assumption that small-scale yielding does not hold in the non-irradiated case. In fact, the plastic zone size in the non-irradiated case is about 24 times as large as that in the irradiated case at the same condition of $K = 30$ MN/m$^{3/2}$. Hence, the condition of small-scale yielding is no longer satisfied in the non-irradiated case.

In the irradiated case, on the other hand, the calculated results seem to be feasible, because both results agree well with each other.

5. Summary and conclusions

1. The comparison between the theoretical model and the FEM simulation was made in terms of film rupture strain.
2. In the irradiated case the crack growth rates of the theory agree well with those of FEM, with the relation of

   $$\varepsilon_{\mathrm{f\ Theory}} = 3.1\varepsilon_{\mathrm{f\ FEM}}.$$

3. In the non-irradiated case, however, the crack growth rates of the theory do not agree with those of FEM.

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