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ARTICLE

Influence of Randomness on Mechanical Properties at Tip of Stress Corrosion Cracking in Nickel-Based Alloys

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Abstract: Stress corrosion cracking (SCC) in nickel-based alloys is one of the most important potential safety hazards in primary circuit of nuclear power plants. Considering the randomness of physical parameters and based on the theory of oxide film rupture, the dispersion law of mechanical properties at SCC tip of nickel-based alloys was studied. To improve the efficiency of numerical analysis with random parameters, combining the advantages of MATLAB and sub-model technology of ABAQUS, MATLAB was employed in the secondary development for ABAQUS. With the help of finite element numerical simulation and Latin hypercube sampling (LHS) method, the effect of random parameters such as Young's modulus and yield strength on the stress and strain of the oxide film region and the base metal region was investigated. Meanwhile, the feasibility of the method was verified. The results show that the influence of randomness should not be ignored. The randomness of yield stress has the greatest influence on the dispersion of stress at SCC tip, and the randomness of Young's modulus has the most significant effect on the plastic strain dispersion at SCC tip.

Key words: nickel-based alloy; stress corrosion cracking; Latin hypercube sampling; uncertainty

Due to good corrosion resistance and mechanical property in high temperature and pressure water environment, nickel-based alloys and austenitic stainless steels are widely applied to the components of primary circuit in nuclear power plants, but SCC of nickel-based alloys and austenitic stainless steels is one of the major factors that affect the reliability and integrity of the nuclear power plants[1,2].

Since SCC is an important degradation mechanism affecting the structural materials of nuclear power plants, dozens of models are constructed to understand the mechanism of SCC, of which the slip/dissolution oxidation model has been widely accepted as a reasonable description of SCC in an oxygenated aqueous system[3,4]. In this model, the strain rate at the cracking tip is the main mechanical factor, so the stress state at the cracking tip is very important, and many attempts have been made to acquire the mechanical state[5,6]. However, the uncertainty of mechanical properties at SCC tip has rarely been researched. Studies show that geometrical and physical random parameters of the structure with crack, such as material property and geometrical dimension of structure strongly influence the fracture parameters[7]. In recent years, research has shown that an analytic method is able to calculate the randomness of fracture parameters considering geometrical parameters and load as random parameters. Because of the complexity at the cracking tip, it is very difficult to consider all the parameters as random variables when analyzing the mechanical properties using a method[8]; meanwhile, it is difficult to satisfy the complex structure by tradition Monte Carlo (MC) method with a large amount of computation work. In order to solve the problem, several methods have been proposed. Among them, Latin hypercube sampling (LHS) method as a numerical method is extensively used to deal with structure reliability and nonlinearity issues because the random variable can be considered[9,10], but it is still rarely applied to solve the problem of mechanical properties at SCC tip.

The main purpose of this study is to analyze the effect of randomness on the mechanical properties at SCC tip based on the slip/dissolution oxidation model and the LHS method,

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which provides a method to improve the prediction accuracy of SCC growth rate of nickel-based alloys in the important structure of nuclear plants.

1 Theoretical Basis

1.1 Oxide film rupture theory

SCC is a micro fracture process that occurs at the cracking tip under combined action of mechanics, materials and environment. Therefore, the mechanical field at SCC tip is very important. Micro-model of SCC structure is shown in Fig.1. According to the oxide film rupture theory, a dense oxide film is formed on the surface of the metal by oxidation reaction with the medium environment. Oxide film is partial for some reason, and the exposed metal is used as an anode relative to the oxide film. A great current is generated by the small area of the anode, and it results in the rapid dissolution of the metal. So the crack forms and propagates along the crystal, as shown in Fig.1a. According to FRI model, the SCC growth rate of nickel-based alloys in high temperature water environment can be expressed as[11]:

$$\frac{\mathrm{d}a}{\mathrm{d}t}=\kappa_a^{'}\cdot\left(\frac{\mathrm{d}\varepsilon_\mathrm{p}}{\mathrm{d}a}\right)^{1/(1-m)} \tag{1}$$

where, $\kappa_a^{'}$ is SCC tip oxidation rate constant, which depends on the electric-chemical environment and material in cracking tip area. $\mathrm{d}\varepsilon_\mathrm{p}/\mathrm{d}a$ is the variation of tensile plastic strain with crack growth at a characteristic distance r_0 in front of the cracking tip, and m is the exponent of the current decay curve in the cracking tip. Effect of the micro-mechanical state at the cracking tip on SCC growth process can be illustrated in Fig.1b. In this paper, the cracking tip is simplified to passivation circle, the direction of crack propagation is horizontal, and the stress of material is vertical.

1.2 Latin hypercube sampling method

Because of its efficient stratification properties, LHS is primarily intended for use with long-running models[10]. In view of the complexity of mechanical properties at SCC tip in nickel-based alloys, LHS is adopted to analyze the randomness of it.

It is a stratified-random procedure that LHS provides an efficient way of sampling variables from their distributions. If LHS involves sampling *ms* values from the prescribed distribution of each of n variable X_1, X_2, ... X_n, and it is assumed that the variables are independent of each other, the procedure of LHS is as follows:

1) Divide the cumulative distribution of each variable into m equiprobable intervals, and then, select a value randomly from each interval. For example, random stratified sampling of variable x_1 and x_2 at five intervals, as shown in Fig.2a. For the ith interval, the sampled cumulative probability P_i can be denoted as:

$$P_i=\frac{1}{m}r_\mathrm{u}+\frac{i-1}{m} \tag{2}$$

where, r_u is uniformly distributed random number ranging from 0 to 1.

2) Transform the cumulative probability P_i into the value x with the inverse of the distribution function Q^{-1}:

$$x=Q^{-1}(P_i) \tag{3}$$

3) The N sampling values is obtained through the method that each variable x is paired randomly with *ms* values of the other variables. For Fig.2 example, the Latin hypercube sampling of variable x_1 and x_2 is shown as Fig.2b.

2 Analysis on Mechanical Properties with Random Variable

2.1 Specimen model

To analyze the effect of random variable on mechanical

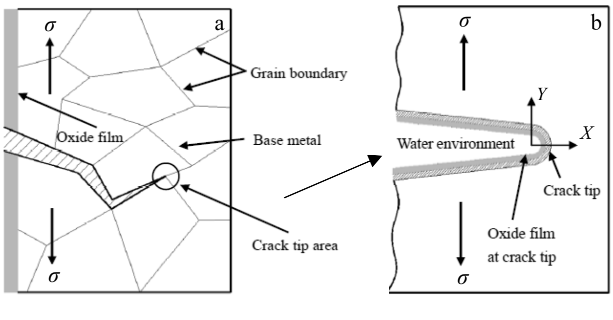

Fig.1 Diagrams of SCC intergranular propagation (a) and SCC tip (b)

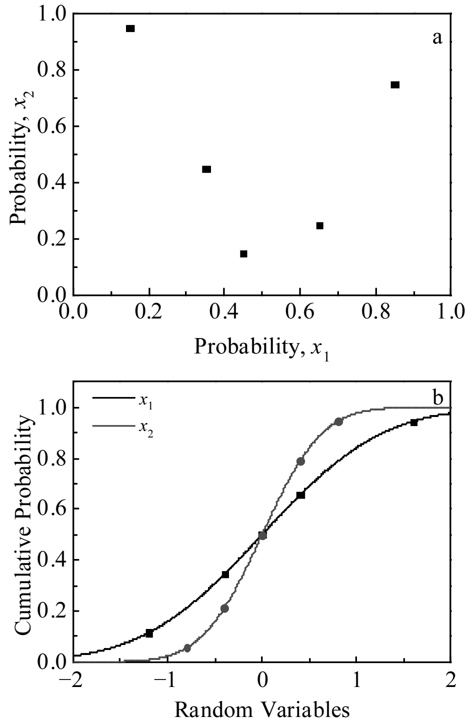

Fig.2 Example of LHS: (a) random stratified sampling and (b) Latin hypercube sampling

properties at SCC tip, a numerical simulation of SCC tip is performed for nickel-based alloys in a simulated oxygenated high-temperature (288 °C) water environment.

One inch compact tension (1T-CT) specimen under a simple tensile load is usually used in SCC experiments in simulated high temperature water environment, whose geometric shape and size are shown in Fig.3a. Therefore, 1T-CT specimen is adopted as the basic analysis object in the research, and it is assumed that the virtual experiment process accords with the American Society for Testing and Materials (ASTM) Standard E399[12].

Taking into account that the state of SCC tip in nickel-based alloy and oxide film is different, two observation paths are adopted at the SCC tip. Path 1 is nearby the oxide film surface and path 2 is nearby base metal, which is shown in Fig.3b. Assuming that the x axis is horizontal and the y axis is vertical, the direction of crack propagation is 0° and the direction of load is 90°. In high temperature and high pressure water, the thickness of oxide film of nickel-based alloy is about 2 μm[13].

2.2 Material and finite element model

The main purpose of this study is to evaluate the effect of material's randomness on the mechanical properties at SCC tip of nickel-base alloys. The nickel-based alloy 600 is used as the basic material, and it is assumed that the stress-strain relation of SCC tip of alloy 600 is represented as Ramberg-Osgood equation in the numerical simulation.

Some important material parameters including Young's modulus, Poisson's ratio and yield strength of alloy 600 and oxide film are described as normal distribution parameters. For simplicity, the variation coefficient of all the random variables (the ratio of mean square variance to mean) are assumed as 0.1 and all random variables are mutually independent[8]. Table 1 shows the mean values of material parameters of nickel-based alloys and oxide film in pressurized water reactor (PWR).

To derive the text file of the .rpy and the .dat which is needed to secondary development for ABAQUS with MATLAB, a commercial finite element model code ABAQUS is used in this simulation analysis when all the random variables are mean. The concentrated loads are applied on the up and down pin

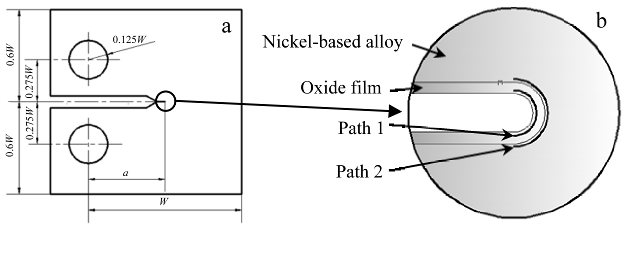

Fig.3 Specimen model: (a) geometrical shape and size of 1T-CT specimen (W=50 mm, a=0.5W, c=1.6 mm) and (b) SCC tip and measured paths

Table 1 Mean values of mechanical properties of alloy 600 and oxide film in PWR environment[14]

Material	Alloy 600	Oxide film	Distribution
Young's modulus, E/GPa	189.5	140	Normal
Poisson's ratio, ν	0.286	0.31	Normal
Yield strength, σ_0/MPa	436	-	Normal
Yield offset, α	3.075	-	-
Hardening exponent, n	6.495	-	-

holes, which keep the stress intensity factor K_{I} of 20 MPa·m$^{1/2}$[5]. Mesh of specimen is shown in Fig.4a, and 8-node biquadrate plane strain quadrilateral elements are adopted in this model. In order to observe and study the detailed stress and strain state in the vicinity of SCC tip, the mesh at the cracking tip region is refined, as shown in Fig.4b.

2.3 Secondary development for ABAQUS

The random analysis with LHS method needs multiple sampling. To improve the effectiveness of simulation with finite element software ABAQUS, MATLAB is employed to develop pre-processing and post-processing. The procedure of ABAQUS is shown in Fig.5.

When the user constructs model and visual processing of the analysis with ABAQUS/CAE, every operation command is recorded in .rpy file of ABAQUS which can change the

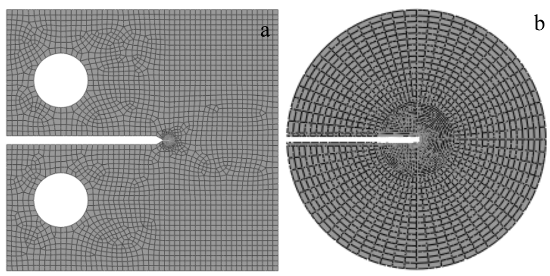

Fig.4 Finite element mesh of 1T-CT specimen: (a) whole model and (b) detail around cracking tip

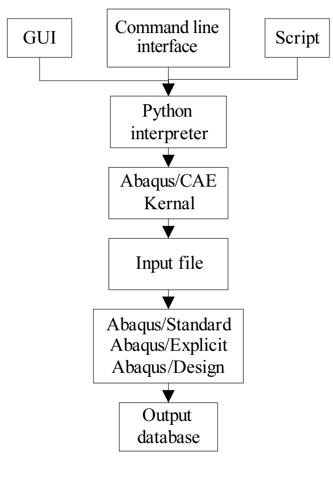

Fig.5 Procedure of ABAQUS

suffix name to .py. The .py file is a text file. In addition, the .inp file which is used in submitting task analysis and the .dat file which is generated by ABAQUS are text files too. Since MATLAB software can modify the text file, it can be employed to develop pre-processing and post-processing program of ABAQUS[15]. The block diagram of joint program of MATLAB and ABAQUS with LHS method is shown in Fig.6, and the process is as follows:

1) Determine the statistic characteristic of each random variable. If the random variable is not normal distribution, it should be converted into normal distribution variable using equivalent normalization method;

2) Generate random variables sets with LHS method, and the sample size is 400[16];

3) Program with MATLAB. The .py file of ABAQUS is called to realize the replacement of random variables;

4) Calculation and analysis with ABAQUS, and return the calculated value of response quantity in result file .dat to MATLAB;

5) The statistical characteristics are obtained by statistical analysis of the calculated response value.

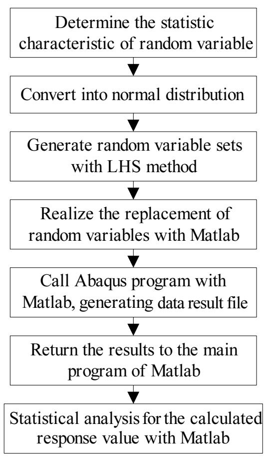

Fig.6 Block diagram of joint program of MATLAB and ABAQUS

3 Results and Discussion

3.1 Effect of randomness on tensile stress

The tensile stress along path 1 and path 2 considering the random parameters are shown in Fig.7 and Fig.9, respectively. The deterministic result is a certain value in the random result, which cannot completely describe the law of the tensile stress with crack angle, so influence of randomness on tensile stress cannot be ignored. The variation trend of the maximum, the minimum and the mean tensile stress with crack angle is basically similar. From Fig.7, it can be seen that at SCC tip of −90°~90°, the variation trend of tensile stress with crack angle is approximately symmetric distribution of 0° direction. At the SCC tip of about 0°~60°, with the increasing of crack angle, tensile stress increases gradually, and at the SCC tip of 60°~90°, with the increasing of crack angle, tensile stress decreases gradually, which indicates that the tensile stress corrosion along path 1 is easy to be generated at SCC tip of about 60°. From Fig.9, it can be seen that the minimum tensile stress appears at the vicinity of 0° direction because of the constraint effect of SCC tip. Comparing Fig.7 and Fig.9, the tensile stress in the oxide film is much larger than that in the nickel-based metal, which implies that the oxide film rupture may play a more important role in the SCC.

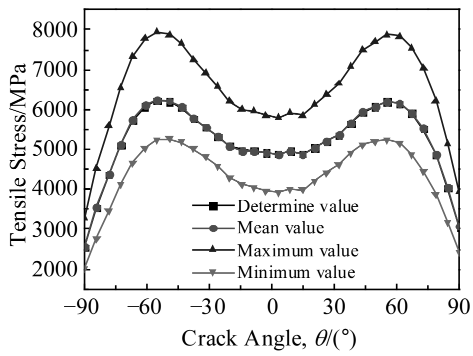

Fig.7 Tensile stress along path 1

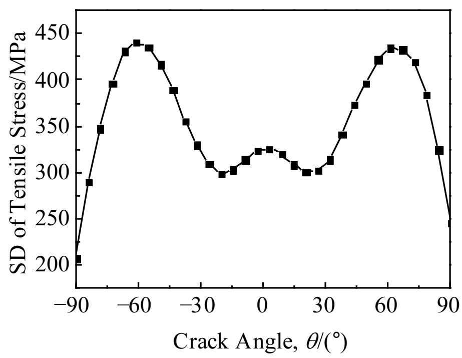

Fig.8 SD of tensile stress along path 1

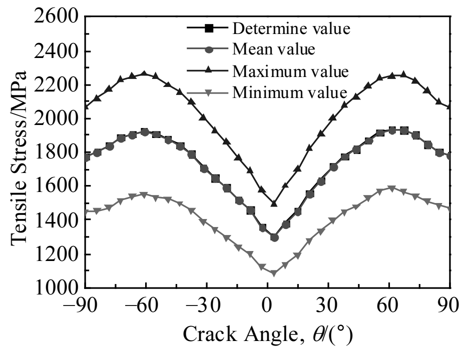

Fig.9 Tensile stress along path 2

Standard deviation (SD) of tensile stress along path 1 and path 2 considering the random parameters are shown in Fig.8 and Fig.10, respectively. At the SCC tip of 0°~30°, the maximum SD of tensile stress along path 1 is at 0°. At the SCC tip of 30°~90°, the maximum SD of tensile stress along path 1 is at the vicinity of 60°, as shown in Fig.8. At the SCC tip of 0°~90°, the maximum SD of tensile stress along path 2 is at the vicinity of 60°, as shown in Fig.10.

3.2 Effect of randomness on tensile plastic strain

The tensile plastic strain along path 2 considering the random parameters are shown in Fig.11. The variation trend of the maximum, the minimum and the mean tensile stress with crack angle is basically similar. Tensile stress plastic strain with crack angle is approximately symmetric distribution of 0° direction. At the SCC tip of 0°~30°, with the increasing of crack angle, tensile stress increases gradually, and at the SCC tip of 30°~90°, with the increasing of crack angle, tensile stress decreases gradually.

SD of tensile plastic strain along path 2 considering the random parameters is shown in Fig.12. The dispersion of tensile stress with crack angle is approximately symmetric distribution of 0° direction, too. At the SCC tip of 0°~60°, the maximum dispersion of tensile plastic strain appears at the vicinity of 30°, which implies that the calculation deviation caused by random factors at the direction is larger than those at other directions.

3.3 Effect of randomness at the SCC tip

To verify the correctness of the proposed method, MC method after 5000 simulated sampling is used to obtain the mechanical properties. SD_{all} takes all the random variable into consideration using LHS method and MC method. From the result of second and third columns in Table 2, we can observe that the SD of mechanical properties using LHS and MC method is very similar, which implies that the proposed method has certain rationality and calculation precision.

To analyze a single random effect on the mechanical properties at SCC tip of nickel-based alloys, the Young's modulus, Poisson's ratio and yield strength of alloy 600 and oxide film are separately considered, and the coefficient of each variation is the same as 0.1. SD_{E1}, $SD_{\nu1}$, $SD_{\sigma0}$, SD_{E2} and $SD_{\nu2}$ are the SD of mechanical properties at SCC tip with respect to each random variable. Where, the lower corner mark E_1, ν_1 is the Young's modulus and Poisson's ratio of alloy 600, while E_2, ν_2 is the Young's modulus and Poisson's ratio of oxide film.

From the result of Table 2, we can observe that dispersion of yield strength has the greatest effect on the SD of tensile stress along path 1 and path 2, Young's modulus comes second, and Poisson's ratio has the lowest effect. In addition, the effect of E_1 uncertainty on SD of tensile plastic strain along path 2 is the greatest, and the yield strength comes second.

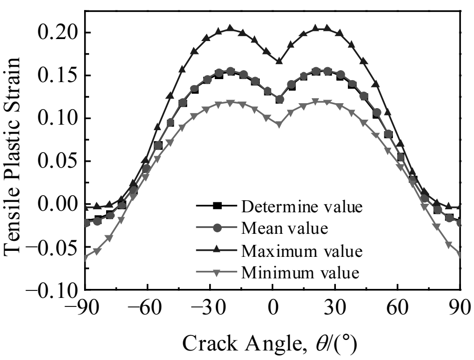

Fig.11 Tensile plastic strain along path 2

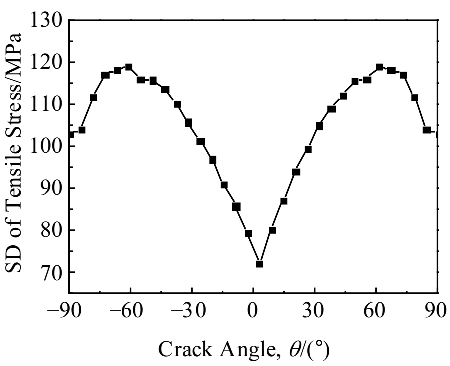

Fig.10 SD of tensile stress along path 2

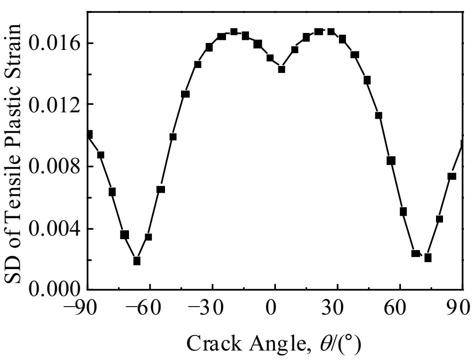

Fig.12 SD of tensile plastic strain along path 2

Table 2 SD of mechanical properties by proposed method and the contribution to SD of each random variable

Location	SD_{all} (LHS)	SD_{all} (MC)	SD_{E1}/GPa	$SD_{\nu1}$	$SD_{\sigma0}$/MPa	SD_{E2}/GPa	$SD_{\nu2}$
Path 1-S22	325.861	323.824	22.793	22.005	316.216	23.497	8.808
Path 2-S22	72.169	71.631	11.092	4.172	69.759	12.160	2.046
Path 2-PE22/$\times10^{-2}$	1.434	1.396	1.111	0. 205	0. 737	0. 046	0. 019

4 Conclusions

Based on the LHS method and elastic-plastic finite element method, an approach is proposed to achieve the random effect on the mechanical properties at SCC tip of nickel-based alloys in high temperature water environment. This approach can be used to understand the dispersion of stress and strain in the SCC tip of important structure in nuclear power plant. According to this approach, the following conclusions are obtained:

1) Due to the randomness of physical parameters, the uncertainty of mechanical properties at SCC tip should not be ignored. The deterministic result which is a definite value among random value is similar to the mean value, but it cannot completely describe the law of mechanical properties.

2) Combined with the advantages of MATLAB and ABAQUS, the program of mechanical properties of SCC tip calculated by MATLAB-ABAQUS is compiled based on LHS method, and the proposed method has certain rationality through the comparison of MC method.

3) Among the physical random variables, dispersion of yield strength has more significant influence on the SD of tensile stress, which indicates that the uncertainty of yield strength should be minimized first in order to improve the tensile stress of SCC tip. However, dispersion of Young's modulus has more significant influence on the SD of tensile plastic strain, so the smaller the dispersion of Young's modulus is, the less the fluctuation of SCC growth rate is.

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随机因素对镍基合金应力腐蚀裂尖力学特性的影响

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摘 要：镍基合金的应力腐蚀开裂是核电站一回路中最重要的潜在安全隐患之一，考虑物理参数的随机性，基于氧化膜破裂理论，研究了镍基合金应力腐蚀裂尖力学特性的分散性规律。为了提高随机参数数值分析的效率，结合 MATLAB 和 ABAQUS 子模型技术的优点，完成了 MATLAB 对 ABAQUS 的二次开发，将有限元数值模拟和拉丁超立方抽样（LHS）方法相结合，获得了弹性模量、屈服强度等随机参数对应力腐蚀裂尖氧化膜和基体金属区域应力应变的影响规律，并验证了方法的可行性。结果表明，随机性的影响不容忽略，屈服应力的随机性对裂尖应力的分散性影响最大，而弹性模量的随机性对裂尖塑性应变分散性的影响最为显著。

关键词：镍基合金；应力腐蚀开裂；拉丁超立方抽样；不确定性

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