Simulation of Creep Crack Propagation and Life Assessment of GH3535 Alloy Based on Fracture Mechanics

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Abstract

Within the Thorium Molten Salt Reactor (TMSR), a fourth-generation advanced reactor, lifetime prediction of high-temperature components containing defects constitutes a crucial component of structural integrity assessment. In this study, firstly, based on time-dependent creep fracture mechanics, the creep fracture parameter C* was calculated utilizing the contour integral method in the finite element analysis software Abaqus. In conjunction with an automated analysis program developed in Python, creep crack growth (CCG) in GH3535 alloy compact tension specimens C(T) was predicted. Numerical calculation results were compared and validated against creep crack growth experimental data, with sources of uncertainty in the numerical simulations analyzed. Subsequently, a Time-Dependent Failure Assessment Diagram (TDFAD) for GH3535 alloy was established, and the stress intensity factor K and reference stress during the crack propagation process were extracted and calculated from finite element results. Finally, lifetime assessment was conducted on defective specimens. In creep crack growth numerical simulations, the creep fracture parameter C* can only characterize the crack propagation stage, whereas the crack initiation stage was described using crack initiation time fitted from experimental data. The lifetime of high-temperature defective structures is correlated with factors such as defect dimensions, loading, and crack growth rate, whose influences can be obtained through numerical simulation methodologies. The research findings elucidate the creep crack behavior of GH3535 alloy and provide engineering guidance for lifetime prediction of high-temperature defective structures in TMSR.

Full Text

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Abstract

Life prediction of high-temperature defective components represents a critical aspect of structural integrity assessment in the thorium molten salt reactor (TMSR), a fourth-generation advanced reactor system. This study aims to simulate creep crack growth (CCG) in compact tension C(T) specimens and conduct life assessment, providing engineering guidance for life prediction of defective structures at elevated temperatures in TMSR. The research first simulated CCG in C(T) specimens using the contour integral evaluation method in finite element analysis (FEA). An automated analysis program written in Python was developed based on time-dependent creep fracture mechanics to calculate the creep fracture parameter C. *A time-dependent failure assessment diagram (TDFAD) for GH3535 alloy was established, and the stress intensity factor K and reference stress were extracted and calculated from FEA results. Finally, life assessment was performed on a C(T) specimen. Comparison between experimental data and simulation results using the creep fracture parameter C* demonstrates that the FEA method can effectively simulate crack propagation in specimens. The TDFAD of GH3535, combined with FEA, visually presents the process of crack propagation leading to equipment failure. The research results elucidate the creep crack behavior of GH3535 alloy and provide engineering guidance for life prediction of defective structures at elevated temperatures in TMSR, ensuring the safety and reliability of the reactor' s high-temperature components.

Keywords: GH3535, Creep crack propagation, Defect assessment, Thorium molten salt reactor (TMSR)

Introduction

Molten salt reactors represent one type of fourth-generation nuclear fission reactor receiving significant international attention. During the 1950s-60s, Oak Ridge National Laboratory (ORNL) developed the structural material UNS N10003 alloy for molten salt reactors. However, ORNL reports indicated cracking issues in welded specimens of Hastelloy N alloy (the UNS N10003 alloy produced by Haynes International) [1]. In the Thorium Molten Salt Reactor (TMSR) program, UNS N10003 alloy has been successfully domesticated in China. The mechanical properties and molten salt corrosion resistance of the domestic UNS N10003 alloy (designated GH3535) have been experimentally proven to be comparable to imported Hastelloy N alloy [2], although GH3535 alloy exhibits certain welding crack sensitivity [3,4]. The presence of cracks in the alloy poses potential hazards and adverse effects on the long-term service life and structural integrity of components.

For crack propagation in metals at high temperatures, some scholars have developed creep damage models based on continuum damage mechanics theory to predict creep crack growth. Wang et al. [5] established a numerical simulation method to predict creep crack growth in UNS N10003 alloy based on the Liu and Murakami (L-M) creep damage model. On the other hand, metal structure defect assessment codes developed according to the "fitness-for-service" principle, such as the British power industry standard R5 [6], British national standard BS7910 [7], and Appendix A16 of the French RCC-MR code [8], are mostly based on linear elastic fracture mechanics (LEFM) and the creep crack growth rate (CCGR) method. The CCGR method determines the relationship between crack length and time under creep conditions through testing, then calculates the crack growth rate using finite element analysis combined with material performance parameters [9,10]. To apply these metal structure defect assessment codes in engineering practice, it is necessary to establish corresponding finite element analysis models and applicable life assessment methods for GH3535 alloy. The time-dependent failure assessment diagram (TDFAD) method, developed by Xuan et al. [11–13] based on international high-temperature defect assessment codes, represents a three-level assessment method for high-temperature applications suitable for GH3535 high-temperature alloy structural defect assessment.

This study, based on time-dependent creep fracture mechanics, developed an analysis program using the contour integral method in finite element analysis software Abaqus to predict the creep crack growth behavior of GH3535 alloy compact tension (C(T)) specimens at 650°C under different loads, and employed the TDFAD method to conduct life assessment of defective specimens.

1. Material Parameters and Mechanical Test Data

The nickel-based superalloy GH3535 is an austenitic γ-phase alloy containing numerous precipitates (M6C-type carbides) within grains and at grain boundaries. The operating temperature of molten salt reactors is 650°C, and relevant material testing has been conducted at the Shanghai Institute of Applied Physics. At 650°C, GH3535 alloy has a Young' s modulus of 178 GPa, Poisson' s ratio of 0.34, yield strength of 174 MPa, and true tensile strength of 596 MPa. Wang et al. [14] fitted the material constants for the Norton model and Kachanov-Rabotnov (K-R) model using uniaxial tensile test data of GH3535 alloy smooth round bar specimens at 650°C. This study adopts the Norton model fitting results and discusses the applicability of other models.

Creep crack growth test data were obtained from the results of Fan et al. [15], who conducted creep crack growth tests on C(T) specimens at 650°C according to the ASTM E1457 standard [16]. The tests included three specimens: CT12, CT13, and CT14, with initial crack lengths of 10.16 mm, 10.20 mm, and 10.20 mm, respectively. The crack initiation time was defined according to ASTM E1457 as the test time when the creep crack growth increment reached 0.2 mm, which were 432 h, 615 h, and 909 h, respectively. The total crack growth increments were 1.48 mm, 1.01 mm, and 1.60 mm, and the total test durations were 860 h, 1122 h, and 2254 h, respectively. Through these tests, the numerical fitting relationship between creep crack growth rate and fracture mechanics parameter C* for GH3535 at 650°C was obtained, i.e., the creep crack growth rate equation: $\dot{a} = 0.0199(C^*)^{0.89}$, where $\dot{a}$ is the creep crack growth rate ($\mathrm{mm} \cdot \mathrm{h}^{-1}$) and C* is the fracture parameter ($\mathrm{N} \cdot \mathrm{mm}^{-1} \cdot \mathrm{h}^{-1}$).

2.1 Finite Element Analysis Method

The finite element simulation model adopted the specimen parameters from Fan et al. [15], establishing a two-dimensional model in Abaqus software. The actual thickness of the specimen was assigned in the section properties, and an initial crack was pre-set at the crack front using Abaqus' s seam function. Reference points RP-1 and RP-2 were defined at the centers of the two loading holes and coupled with the corresponding hole perimeters through rigid constraints. Following the actual test conditions, reference point RP-2 was fixed, and the test load was applied at reference point RP-1. The specific loads and boundary conditions are shown in [Figure 1: see original paper] (left). The analysis consisted of two load steps: Step-1 performed static calculation, and Step-2 performed visco calculation considering creep effects on the crack.

Model meshing was controlled through self-written Python code. The meshing strategy involved setting multiple circular mesh regions at the crack tip, with the remaining portions divided into regular geometric blocks for automatic meshing by Abaqus. This approach facilitates Abaqus' s calculation of the creep fracture parameter Ct-integral using the contour integral method. As the crack propagated, the model and mesh evolved over time. The mesh type was 8-node quadrilateral shell elements (CPS8), with element numbers varying between 1,900 and 4,000. A schematic of the finite element analysis model is shown in [Figure 1: see original paper] (right). Local refinement was applied to the crack tip region. When the circular arcs were divided using 30, 40, and 50 nodes, the relative error of the global maximum Mises stress was 0.1%, and the relative error of the creep fracture parameter Ct-integral was less than 0.1%. When the innermost mesh size at the crack tip was 0.02 mm, 0.04 mm, and 0.08 mm, the relative error of the global maximum Mises stress was less than 0.1%, and the relative error of the Ct-integral was less than 0.1%. The mesh independence of the model calculation results was thus verified.

The Python code analysis program also calculated the crack extension amount and determined the crack propagation direction based on the obtained fracture parameter C* combined with creep crack growth test results, then reconstructed a new model. The program repeated this process after obtaining new parameters from subsequent calculations. The program analysis flowchart is shown in [Figure 2: see original paper]. The fracture parameter C* was taken as the value when the Ct-integral reached the fracture time t_f, where t_f is the time corresponding to when the maximum creep strain in the model reached the creep fracture strain ε_f. The crack propagation direction was determined using the maximum stress criterion, selecting the grid unit point with maximum stress at the crack tip.

2.2 Calculation Results

This study achieved dynamic crack propagation simulation using the program, presenting the gradual increase in crack size over time. Partial screenshots of the crack tip region from the finite element simulation results for specimen CT13 are shown in [Figure 3: see original paper]. In the finite element calculation results, the maximum Mises stress at integration points equals the material' s tensile strength, but the data displayed in the Mises stress contour plot in [Figure 3: see original paper] shows nodal values. Nodal values are extrapolated from integration points based on element type, which is why the contour plot shows maximum Mises stress slightly higher than the material' s tensile strength. A comparison between experimental data and simulation results for the three specimens is presented in [Figure 4: see original paper].

Only cases with crack growth increments greater than 0.2 mm were selected for comparison in [Figure 4: see original paper]. This is because the creep crack growth rate equation obtained from tests only considered data after crack initiation time $t_{0.2}$, i.e., only test results after the crack growth increment reached 0.2 mm were considered. Therefore, the same treatment was applied to numerical simulation results: data before the crack growth increment reached 0.2 mm in the simulation were discarded, and the time was reset to the crack initiation time $t_{0.2}$.

The comparison between experimental data and simulation results demonstrates that this finite element analysis method can effectively simulate crack propagation in specimens. The simulation results are slightly larger than the experimental data, which is conservative for subsequent life assessment of defective structures using the simulation results.

Additionally, when using other material constitutive models besides the Norton model for creep analysis, such as the K-R model or Liu and Murakami (L-M) model, the computational time step becomes smaller and the time consumption increases significantly. For example, the K-R model increases computation time by approximately 115 times. Both the K-R and L-M models are creep damage models based on continuum damage mechanics. Since this study conducts crack propagation simulation based on fracture mechanics, using creep damage models may lead to increased computational costs.

3.1 Time-Dependent Failure Assessment Diagram

According to the secondary failure assessment curve in R6 [17], the failure assessment curve is defined as follows:

$$L_r = \frac{\sigma_{ref}}{\sigma_y}$$

$$K_r = \frac{K}{K_{mat}}$$

where L_r is the ratio of applied load to structural limit load; K_r is the ratio of stress intensity factor K to material creep fracture toughness K_{mat}; σ_{ref} is the reference stress (MPa); σ_y is the yield strength (MPa); and E is Young' s modulus (MPa).

The maximum allowable limit $L_{r(max)}$ is defined as:

$$L_{r(max)} = \min\left(\frac{\sigma_{ref}}{\sigma_y}, \frac{\sigma_{ref}}{0.2\% \text{ proof stress}}, \frac{\sigma_{ref}}{\sigma_{UTS}}\right)$$

where σ_{UTS} is the ultimate tensile strength (MPa), and the 0.2% proof stress is the stress corresponding to 0.2% strain on the stress-strain curve at t=0.

Using the isochronous stress-strain curves of GH3535 at different times, the failure assessment diagram was established as shown in [Figure 5: see original paper]. Taking specimen CT12 as an example for life assessment, the trajectory of (K_r, L_r) during crack propagation was plotted in [Figure 5: see original paper]. The figure shows that this specimen cannot meet the safety requirement for a 10,000-hour life, and with further crack propagation, it will exceed the failure assessment curve for a 1,000-hour life. The total test duration for this specimen was 860 h, which basically matches the life prediction for specimen CT12 in this study.

3.2 Calculation of Kr and Lr

When assessing component life, K_r and L_r need to be calculated. The stress intensity factor K can be extracted from finite element calculation results. Additionally, L_r is the reference stress ratio. When the material constitutive behavior follows the Norton creep relationship, the following relationship exists [18]:

$$C^* = AK^{n+1}$$

where C* is the fracture parameter ($\mathrm{N \cdot mm^{-1} \cdot h^{-1}}$), K is the stress intensity factor ($\mathrm{MPa \cdot mm^{-1}/^2}$), and A and n are Norton model fitting constants. Therefore, K_r can be extracted from finite element analysis results.

4. Analysis and Discussion

In Section 2.2, we concluded that experimental data and simulation results basically match, with simulation results being conservative. The detailed data comparison is shown in . The table reveals that errors increase over time. The mean absolute errors for the three tests are 0.1339, 0.0929, and 0.1338, respectively, with mean absolute percentage errors (MAPE) of 28.23%, 17.89%, and 25.67%, respectively.

The slightly larger numerical simulation results were analyzed, and the reasons are considered to be as follows:

1. **Inaccuracy of the material creep model**: The Norton model produces more conservative calculation results, which leads to larger creep strain calculations and consequently larger crack growth increment calculations.
2. **Overestimation of the fracture parameter C***: Abaqus calculates the fracture parameter Ct-integral, which reduces to C* when the crack tip region reaches steady-state creep. Some calculation steps may not have reached absolute steady-state creep, resulting in a tendency for C* values to be overestimated.
3. **The creep crack growth rate equation**: This is a mathematical fitting result from three sets of test data, which has different deviations for individual tests, particularly showing a higher deviation for specimen CT-14.
4. **Mesh size and calculation time step**: These factors may also contribute to uncertainties in numerical simulation calculations.

Additionally, this study only simulated and analyzed the creep crack propagation stage. This is because different measurement methods are used for the crack initiation stage and crack propagation stage in creep crack growth tests. The creep fracture parameter C* in numerical simulation can only describe the crack propagation stage, while the crack initiation stage is described using crack initiation time fitted from experimental data. Therefore, the differences between these two stages must be fully considered when conducting life assessment of components.

This study developed an automated analysis program based on finite element analysis software to predict the crack propagation behavior of GH3535 alloy specimens at 650°C and conducted life assessment of defective specimens using the TDFAD method. Experimental data and simulation results basically match, with simulation results being conservative. The research results provide valuable insights for understanding the creep crack behavior of GH3535 alloy and offer practical guidance for monitoring and maintaining in-service GH3535 alloy structures. Furthermore, incorporating time-dependent fracture mechanics will help improve current defect assessment guidelines.

Author Contributions: Wang Wen: literature research, methodology development, program coding, data analysis, writing—original draft; Wang Xiaoyan: data analysis supervision, review and editing; Li Zhijun: topic guidance, experimental support, supervision, review and editing.

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Note: Figure translations are in progress. See original paper for figures.