FEM Analysis of Hydrides at Crack Tip in Zr-2.5Nb Pressure Tube

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1. Introduction

The delayed hydride cracking(DHC) is a unique phenomenon occurred in zirconium alloys. DHC of in Zr-2.5Nb pressure tube is caused by the concentration of hydrogen atoms to the vicinity of a crack tip, nucleation and growth of hydride. After being reported this in the year 1970, AECL etc. have been performed R&D for examining DHC mechanism. Dutton and Puls suggested that the driving force of hydrogen atoms is the tension stress gradient formed at the crack tip[1]. But, this model can't explain Fig.1 and Fig.2 of the unique phenomenon of DHC. At Stage I of Fig.1 and Fig.2, DHC velocity increases quickly and that is constant at Stage II even if the stress intensity factor(K) increases. Also, the striation spacing on the fractured surface of DHC CT(Compact Tension) specimen is firstly wide and becomes gradually narrow according to increasing K value. Finally, that becomes constant at Stage II[2]. The new DHC model suggested in this paper can explain the above phenomena.



Figure 1. Dependence of the crack growth velocity with K



Figure 2. Variation of the striation spacing of DHC

2. Methods and Results

The experimental data[3] is inputed for the FEM model. The stresses of the hydride and Zr-2.5Nb elements near the crack tip of the FEM model are examined. Also, the plastic zone size and average stresses near the crack tip are calculated for checking the effects of the plastic constraint.

2.1 Materials and Specimen

Table 1. Mechanical properties of the Zr-2.5Nb alloy used in the finite element analysis

Elastic Modulus	Poisson's	Yield Strength
(MPa) 250 °C	Ratio	(MPa)
81550	0.329	700

Table 2. Mechanical properties of the hydride



Figure 3. Dimension of CT specimen

2.2 FEM Model

ABAQUS code is used for the FEM analysis. 3D-FEM model includes about 70000 elements of solid linear brick. This model is shown in Fig. 4 and includes a pre-fatigue crack length of 1.7 mm. The element length and thickness of the hydride near a crack tip is 30 μ m and 1 μ m respectively.



Figure 4. 3D Finite Element Modeling of CT specimen

2.3 Hydride expansion stress

When the hydride expands, the increase of the hydride volume is 16%. $X^3+3aX^2+3a^2X=0.16a^3$ Where, a=30 µm. X= ϵ =1. 522 µm. By Hook's law, σ =E. ϵ =131700 × 0.001522= 200MPa. Therefore, when the hydride length of 30 µm grows in X, Y and Z direction, ideally, the hydride expansion stress will be 200MPa. When K_{IH} =7.0 MP \sqrt{m} is applied and the hydride length becomes 30 µm, X direction stress of the Zr-2.5Nb element, which is the next element at the end

of the hydride element, gives a definition of σ_{x1} . When the hydride length becomes 60 µm, X direction stress at the end element of the hydride gives a definition of σ_{x2} . The difference of the two stresses ($\Delta \sigma_x = \sigma_{x2} - \sigma_{x1}$) will be the hydride expansion stress (STEP 1). By the same method, the difference of the two stresses ($\Delta \sigma_x$) is calculated with respect to 60µm (STEP 2) and 90µm (STEP 3) of the hydride length. Results of the analysis are represented in Table 3.

Table 3. Hydride expansion stress in the case of K=7.0MP \sqrt{m}

	σ_{x2}	σ_{x1}	$\Delta \sigma_x = \sigma_{x2} - \sigma_{x1}$
STEP 1	452	331	121
STEP 2	398	307	91
STEP 3	324	243	81

Therefore, the average value of $\Delta \sigma_x$ will be the hydride expansion stress. That is about 100MPa.

2.4 Size of Plastic Zone at Crack Tip

The size of the plastic zone at the crack tip according to each K value is shown in Fig. 5.



Figure 5. Plastic zone size according to each K value

When the K value is 7.79MP \sqrt{m} , the size of the plastic zone at the crack tip becomes constant(45µm) in spite of an increase of the K values. We can establish that K = 7.79MP \sqrt{m} is the transition point of Stage I and Stage II of Fig. 1 and Fig. 2. This implies that the size of the plastic zone on the hydride is the main factor which restrains the growth of the hydride length. Also, this implies that the plastic constraint force is the hydride fracture strength. That is, X direction components of the plastic constraint force are the factor which restrain the growth of the hydride length and Y direction components of that are the hydride fracture strength. The reaction force will exist for the equilibrium of the force between the end of the hydride element and the next Zr-2.5Nb element. The difference of the two stresses ($\Delta \sigma_x = \sigma_{x2} - \sigma_{x1}$) will be the reaction force. Average stresses of the X direction in the plastic zone on the hydride give a definition of $\sigma_{x.ave}$ and those of the Y direction give a definition of $\sigma_{y,ave}$. The values of $\Delta \sigma_x$, $\sigma_{x,ave}$ and $\sigma_{y,ave}$ are represented in Table 4.

Table 4. Reaction force between two elements and the average stresses in the plastic zone

K	$\Delta\sigma_x$	$\sigma_{x.ave}$	$\sigma_{y.ave}$
	(MPa)	(MPa)	(MPa)
7.0	102	-	-
7.44	176	435	802
7.79	618	503	835
8.11	649	496	830
8.37	684	524	868
8.64	679	578	909

In the case of K=7.0 MP \sqrt{m} , there is not almost the plastic zone near the hydride. Therefore, the behavior of the hydride is almost elastic and the value of $\Delta \sigma_x$ is equal to the hydride expansion stress (about 100MPa). $\Delta \sigma_x$ = hydride expansion stress. But, in the case of K=7.79 MP \sqrt{m} , the growth and restraint of the hydride have an influence on the stress created due to the plastic flow. $\Delta \sigma_x$ = hydride expansion stress + $\sigma_{x.ave}$. In the case of higher K values than K=7.79 MP \sqrt{m} , the hydride fracture strength is an average value of $\sigma_{y.ave}$. That is about 860 MPa.

3. Conclusions

1) When the hydride grows to 30 μ m, the hydride expansion stress is about 100 MPa by the FEM analysis.

2) The size of the plastic zone converges into about 45 μ m at higher K values than K=7.79MP \sqrt{m} . The growth and restraint of the hydride have an influence on the stress created due to the plastic flow. When the hydride moves in the plastic zone, the reaction force on the plastic constraint force is generated. Thus, the spacings of the striation lines become constant at Stage II even if K values increases.

3) The hydride fracture strength is about 860 MPa in the case of higher K values than K=7.79 MP \sqrt{m} .

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