

Numerical Study of Coupled Elasto-Plastic Hydrogen Diffusion at Crack Tip Using XFEM



Anjali Jha , I. V. Singh, B. K. Mishra, Ritu Singh, and R. N. Singh

1 Introduction

The mechanical properties and fracture behavior of material are highly influenced by the hydrogen. Hydrogen diffusion in material can cause reduction in tensile strength, failure time, and fracture toughness of the material. The simultaneous process of hydrogen diffusion with hydride precipitation and mechanical deformation is termed as hydrogen embrittlement. Hydrogen embrittlement can reduce the ductility of the material and change the fracture mode from ductile to brittle. The two main mechanisms widely used for the hydrogen embrittlement are hydrogen-induced cohesion and hydrogen-enhanced local plasticity. The later one is used by Sofronis and Mcmeeking [1] where the flow stress of the material is modeled as a function of total hydrogen concentration. Kim et al. [2] used the hydrogen-enhanced plasticity mechanism to analyze the hydrogen transport phenomenon coupled with elasto-plasticity.

The hydrogen present in the environment diffuses inside the material and then follows by precipitation of hydride when the concentration of hydrogen exceeds the terminal solid solubility limit. These hydrides usually precipitate at the high tensile stress regions such as discontinuities and cracks. Hydrides present at the crack tip will grow up to a critical size followed by hydride fracture and then the process repeats. A numerical model is developed which takes into account the processes of

A. Jha (✉) · I. V. Singh · B. K. Mishra
Indian Institute of Technology Roorkee, Roorkee 247667, India
e-mail: ajha3@me.iitr.ac.in

R. Singh
Atomic Energy Regulatory Board, Mumbai 400085, India

R. N. Singh
Bhabha Atomic Research Centre, Mumbai 400085, India

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S. K. Saha and M. Mukherjee (eds.), *Recent Advances in Computational Mechanics and Simulations*, Lecture Notes in Mechanical Engineering, https://doi.org/10.1007/978-981-15-8315-5_16

hydrogen embrittlement to analyze the process of hydrogen diffusion coupled with the material deformation ahead of the crack tip using XFEM [3, 4].

Many researchers have used various methods such as finite element method and cohesive zone modeling to model the hydride-induced cracking. Very few studies are present in which extended finite element is used for this purpose. Shanati et al. [5] used finite element method (FEM) to model the stress-assisted diffusion process and used a staggered approach to solve the coupled problem. Barrera et al. [6] also used FEM to couple the hydrogen diffusion and mechanical behavior of material using coupled temperature displacement process. Kotake et al. [7] studied the fatigue life of a component for transient hydrogen diffusion near the crack tip by coupling the diffusion and plasticity under cyclic loading. The effect of hydrogen diffusion on the yield stress of the material is also considered. Varias and Feng [8] studied the hydride-induced cracking in metals using the finite element method. Martínez-Pañeda et al. [9] used the phase field method to model the hydrogen-assisted cracking in a cracked square plate and notched cylindrical bars.

In the present work, the effects of stress-assisted diffusion on the hydride precipitation and stress triaxiality are studied in the hydrogen environment. The effective plastic strain in the material depends on the stress triaxiality which directly affects the plastic deformation of the material. The stress triaxiality (λ) is defined as the ratio of the hydrostatic stress and the effective von Mises stress. The higher value of stress triaxiality represents the ductile fracture process [10]. The effect of stress triaxiality on edge crack specimen in the presence or absence of hydrogen ahead of the crack tip should be considered. The variation of stress triaxiality with the change in distance from the crack tip is studied.

2 Governing Equations

2.1 Hydrogen Diffusion

The equation of hydrogen diffusion gives the balance of hydrogen in the material at a certain point under steady-state crack growth conditions. It is assumed that no hydrogen is produced within the material. The equation is given as

$$\frac{\partial C^{HT}}{\partial x_1} = \frac{\partial Q_k^H}{\partial x_k} \quad (1)$$

where C^{HT} is the total concentration of hydrogen and Q_k^H is the hydrogen flux. Some of the hydrogen present gets diffused and precipitates in the form of hydrides while the remaining free hydrogen is present in the solid solution. Therefore, the total hydrogen concentration can be written as

$$C^{HT} = fC^{H,hr} + (1 - f)C^H \quad (2)$$

where $C^{H,hr}$ is the concentration of hydrogen in the hydride, C^H is the concentration of hydrogen in the solid solution, and f is the volume fraction of hydrides. The following relation is used to evaluate the hydrogen flux which gives the diffusion of hydrogen in hydrides,

$$Q_k^H = -(1 - f) \frac{D^H C^H}{RT} \frac{\partial u^H}{\partial x_k} \quad (3)$$

where D^H is the diffusivity coefficient and u^H is the chemical potential of hydrogen. The chemical potential of hydrogen depends on the hydrostatic stress in the material,

$$u^H = -\frac{\sigma_{kk}}{3} V^H \quad (4)$$

where V^H is the molar volume of hydrogen and σ_{kk} represents the hydrostatic stress. The evaluated hydrostatic stress is used to solve the diffusion Eq. (1) which requires the gradient of chemical potential of hydrogen and hence the gradient of hydrostatic stress is evaluated as

$$\sigma_{kk,j} = \frac{\partial \sigma_{kk}}{\partial a_p} * J_{ij}^{-1} \quad (5)$$

where J is the jacobian, which maps the natural coordinates with actual coordinates and a_p are interpolation function.

2.2 Hydride Precipitation

The hydrides precipitate in the material when the value of hydrogen concentration in the material exceeds the value of terminal solid solubility C^{TS} ,

$$C^{TS} = C_e^{TS} \exp\left(\frac{\bar{w}_{int}}{mRT}\right) \exp\left(\frac{\sigma_{kk} \bar{V}^H}{3RT}\right) \quad (6)$$

where C_e^{TS} is the terminal solid solubility under no applied stress, m is the hydrogen mole fraction in hydride, and \bar{w}_{int} is the interaction energy of precipitating hydride per mol.

2.3 Material Deformation

Stress field is required to evaluate the hydrostatic stress used in the hydrogen diffusion equation. Therefore, the extended finite element analysis is done to deal with the

hydrogen diffusion crack problem. Elastoplastic analysis is performed to consider the plastic strain around the crack tip. The plastic strain obtained affects the hydrogen diffusion near the crack tip. The constitutive relations used are given as

$$d\sigma_{ij} = D_{ijkl}^{ep} d\varepsilon_{kl} - \frac{E}{3(1-2\nu)} \delta_{ij} d\varepsilon_{mm}^H \quad (7)$$

$$D_{ijkl}^{ep} = \left(\frac{E}{1+\nu} \right) \left[\delta_{ik} \delta_{jl} + \frac{\nu}{1-2\nu} \delta_{ij} \delta_{kl} - \frac{3}{2\bar{\sigma}^2} \times \left(\frac{1}{1 + \frac{2}{3} \frac{dH}{d\bar{\varepsilon}^p} \frac{(1+\nu)}{E}} \right) \sigma'_{ij} \sigma'_{kl} \right] \quad (8)$$

where E is the elastic modulus, ν is Poisson's ratio, δ_{ij} is Kronecker delta, $\bar{\sigma}$ is effective stress, and $\bar{\varepsilon}_p$ is the effective plastic strain. Isotropic hardening of the material is assumed according to the following relations:

$$\bar{\sigma} = H(\bar{\varepsilon}^p) \quad (9)$$

$$\left(\frac{\bar{\sigma}}{\sigma_0} \right)^{1/n} - \frac{\bar{\sigma}}{\sigma_0} = \frac{3E}{2(1+\nu)} \frac{\bar{\varepsilon}^p}{\sigma_0}, \quad \bar{\sigma} \geq \sigma_0 \quad (10)$$

where n is the hardening exponent and σ_0 is the yield strength of the material. Stress trace in the solid solution of the hydride precipitation zone is determined using the following relation [8]:

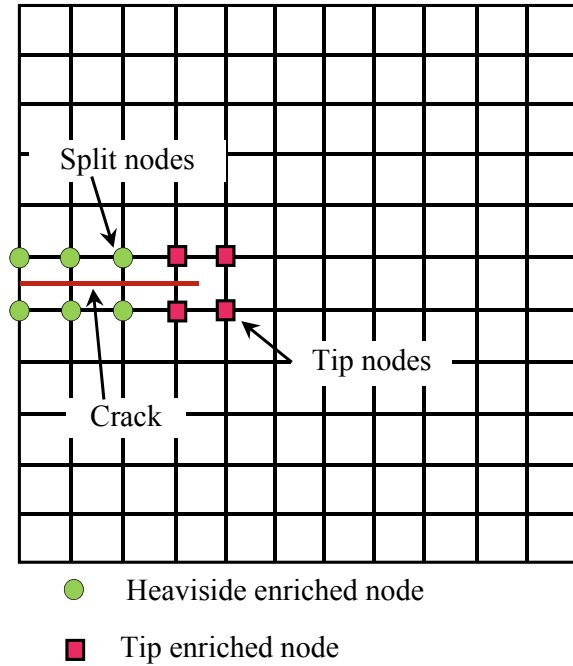
$$\sigma_{kk}^{hz} = \left(\frac{3x}{\theta^{hr} V^{hr}} \right) \left[\frac{\sigma_{kk} V^H}{3} + RT \ln \left(\frac{C_e^{TS}}{C_b^H} \right) \right] \quad (11)$$

where C_b^H and σ_{kk}^{hz} are the concentration of hydrogen and the stress trace of a reference particle, respectively.

3 Methodology

Extended finite element method (XFEM) is used to perform the structural analysis of the model. The XFEM helps in eliminating the issue of re-meshing during crack growth. It is more accurate and requires less computational time as compared to FEM. It uses appropriate enrichment functions in the domain of interest using partition of unity. Heaviside and near tip enrichment functions are used for the elements containing the crack discontinuity as shown in Fig. 1. In XFEM, the enriched displacement approximation can be written as [3]

Fig. 1 Elements intersected by crack with enriched nodes



$$\mathbf{u}^h(\mathbf{x}) = \sum_{i=1}^n N_i(\mathbf{x})\bar{\mathbf{u}}_i + \sum_{i=1}^{n_A} N_i[\mathbf{H}(\mathbf{x}) - \mathbf{H}(\mathbf{x}_i)] \mathbf{a}_i + \sum_{i=1}^{n_B} N_i \sum_{\alpha=1}^4 [F_\alpha(\mathbf{x}) - F_\alpha(\mathbf{x}_i)] \mathbf{b}_i^\alpha \tag{12}$$

where N_i are finite element shape functions, $H(\mathbf{x})$ is a Heaviside enrichment function, and $F_\alpha(\mathbf{x})$ is crack tip enrichment. n is the set of all nodes in the mesh; n_A is the set of nodes associated with those elements which are completely cut by the crack; n_B is the set of nodes associated with those elements which are partially cut by the crack; \mathbf{a}_i is the nodal enriched degrees of freedom for $H(\mathbf{x})$; and \mathbf{b}_i^α is the degrees of freedom vector for $F_\alpha(\mathbf{x})$.

The solution strategy of the model is divided into two parts—diffusion analysis and structural analysis. After giving the initial conditions and properties of the material, structural analysis of the specimen is done to evaluate the hydrostatic stresses in the domain. These stresses are then used to evaluate the hydrogen concentration in the diffusion analysis. If the solution converges, it will be updated at the end of time step. This process continues until the end of time iteration loop. The pre-processing part consists of the evaluation of the hydride fraction, terminal solid solubility, and stress trace and stress triaxiality in the hydride precipitation zone.

An edge crack specimen subjected to tensile loading under plane strain conditions is solved by XFEM. A square-shaped specimen of dimension 2 mm × 2 mm ($L = 2$ mm and $H = 2$ mm) with an edge crack $a = 0.5$ mm is used for the

simulation. The top and bottom edges of the specimen are subjected to a tensile load (σ) of 120 MPa as shown in Fig. 2. x_1 represents the distance from the crack tip in x-direction. A mesh of size (47×47 nodes) is taken for the simulations. Higher order nine node quadrilateral elements are used for the evaluation of the hydrostatic stress gradients. The element containing crack tip is enriched with crack tip enrichment and the elements cut by the crack are enriched with Heaviside enrichment. For the hydrogen diffusion part of the model, a uniform distribution of the hydrogen $C = 6.33 \times 10^5 \text{ mol/m}^3$ is given as the boundary condition. The material properties used are given in Table 1.

Fig. 2 Specimen of edge crack

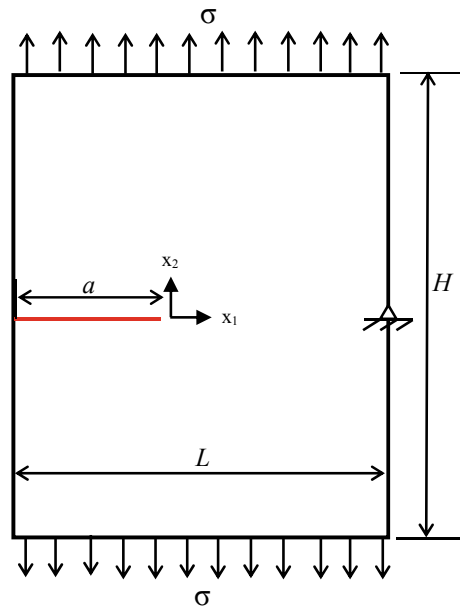


Table 1 Value of material properties correspond to Zircaloy-2 and δ hydride [8]

Material properties	Value
Elastic modulus (E), Poisson ratio (ν)	80.4 GPa, 0.369 (573 K)
Yield strength (σ_{-0})	580 MPa (573 K)
Diffusivity coefficient (D^H)	$2.17 \times 10^{-7} \exp(-35087.06/RT) \text{ m}^2/\text{s}$
Terminal solid solubility (C_e^{TS})	$6.3741 \times 10^5 \exp(-34542.75/RT) \text{ mole/m}^3$
Concentration of hydrogen in hydride ($C^{H,hr}$)	$1.02 \times 10^5 \text{ mol/m}^3$
Molar volume of hydrogen in solid solution (V^H)	$7 \times 10^{-7} \text{ mol/m}^3$
Molar volume of hydrogen in hydride (V^{hr})	$16.3 \times 10^{-6} \text{ mol/m}^3$
Mole fraction of hydrogen in hydride (m)	1.66

4 Results and Discussion

The edge crack specimen is subjected to the tensile loading and the stress–strain behavior of the specimen material predicted is shown in Fig. 3. Stress trace of a reference particle near the crack tip is determined by putting the value of hydrogen concentration in Eq. (11). The value of σ_{kk}^{hz} tends to zero as C_b^H / C_e^{TS} approaches to 1 (hydrogen chemical equilibrium). The results are shown in Fig. 4 and agree well with results available in Varias and Feng [8]. Figure 5 shows the variation of hydride in the edge crack specimen near the crack tip. The hydrogen present in the solid solution will diffuse in the material and hydride precipitates when the hydrostatic stress near the crack tip increases. The volume fraction of hydrogen in hydride is given by hydride fraction (f) whose value varies from 0 to 1. If all the hydrogen is present only in solid solution, then its value is 0 or vice versa. The peak value of hydride fraction is achieved at a small distance from the crack tip where the hydride precipitates and its magnitude increase with the increase in load. Stress triaxiality in the edge crack specimen is also calculated at varying distance from the crack tip (r). As shown in Fig. 6, stress triaxiality increases with increase in distance from crack tip up to a value of 0.08 mm and thereafter it starts decreasing with further increase in r. Higher value of stress triaxiality at the crack tip shows the ductile fracture behavior as suggested by Bao and Wierzbicki [11]. The decrease in stress triaxiality after a distance of 0.08 mm indicates the presence of hydride which reduces the ductility of material ahead of crack tip.

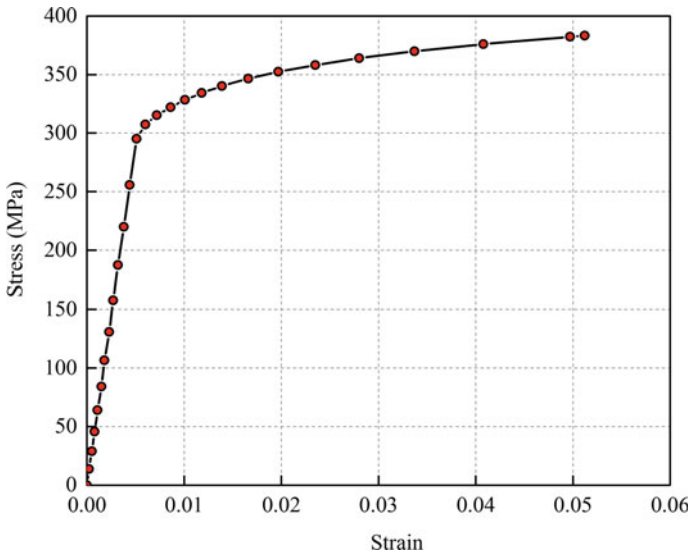


Fig. 3 Stress–strain behavior of the material for Zircaloy-2 at 573 K [8]

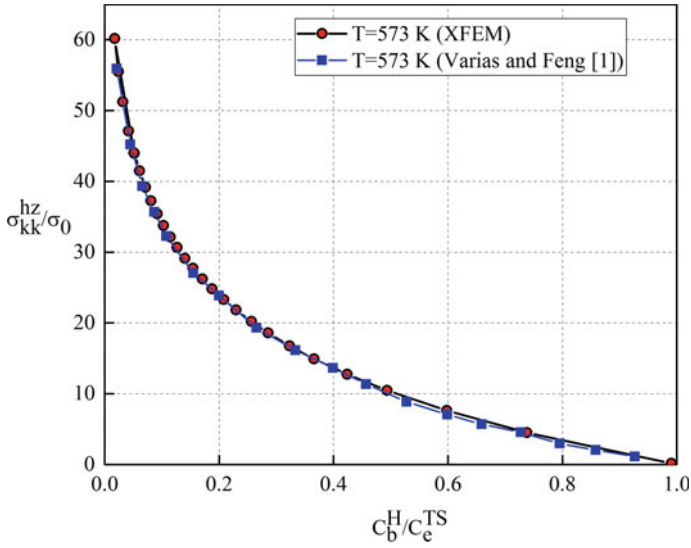


Fig. 4 A comparison of obtained stress trace in the hydride precipitation zone as a function of hydrogen concentration near the crack tip with Varias and Fang [8]

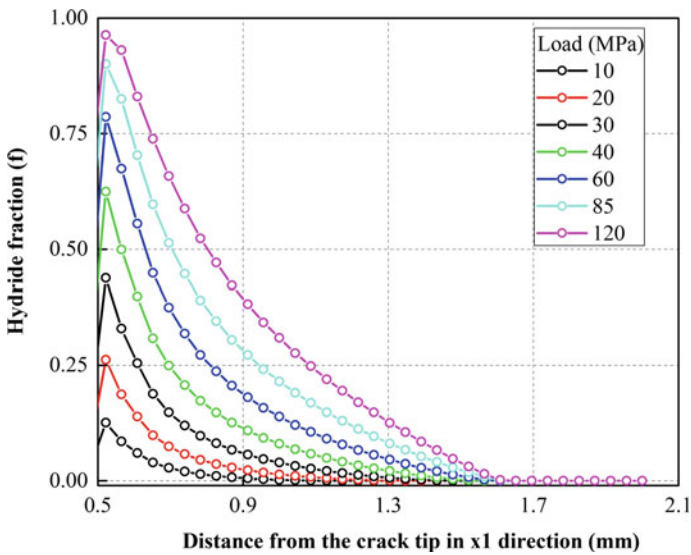


Fig. 5 Hydride fraction with the distance from the crack tip at varying loads

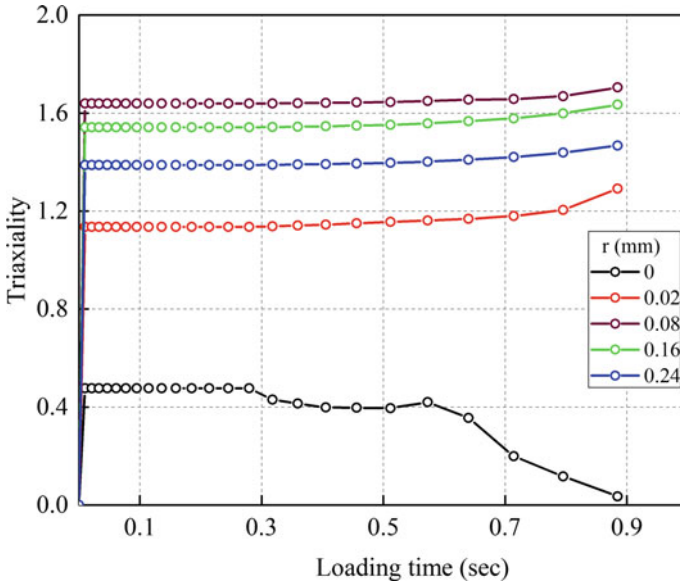


Fig. 6 Variation of stress triaxiality with loading time for different values of distance from the crack tip

5 Conclusion

The hydrogen diffusion coupled with the hydride precipitation and deformation process of the material is modeled for an edge crack specimen using XFEM. Hydrostatic stress is evaluated near the crack tip, and its effect on the hydrogen concentration and hydride precipitation near the crack tip is analyzed. From the present study, the following conclusions can be drawn:

- Hydride fraction increases with increase in load and finally approaches toward its maximum possible value 1.
- With the increase in distance from the crack tip, the hydride fraction first increases to attain a peak value and then decreases.
- The magnitude of peak value of hydride fraction increases with the increase in load.
- Stress triaxiality increases with the increase in distance from the crack tip up to a value of 0.08 and then decreases.

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