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材料氢脆断裂模拟的UEL子程序实现方法 Method for Implementing UEL Subroutine for Simulation of Material Hydrogen Embrittlement

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一、引言 I. Introduction

氢原子进入金属材料内部会恶化其力学性能，主要表现为降低金属材料的使用寿命、塑性变形能力和强度，致使工程结构或构件过早失效，造成灾难性事故。氢脆往往也是指氢原子导致材料的断裂特征从韧性断裂转变为脆性断裂的现象。使用UMAT(User Material Subroutine)子程序及UEL (User Element Subroutine)子程序模拟氢致裂纹扩展行为(HAC, Hydrogen-assisted cracking)目前是有限元模拟方向的热门。本文将总结使用UMAT子程序及UEL子程序来实现氢致裂纹扩展过程模拟的主要原理及方法。

The entry of hydrogen atoms into the internal structure of metallic materials will deteriorate their mechanical properties, mainly manifested as a reduction in the service life, plastic deformation capacity, and strength of metallic materials, leading to premature failure of engineering structures or components and causing catastrophic accidents. Hydrogen embrittlement is often also referred to as the phenomenon where the fracture characteristics of materials are transformed from ductile fracture to brittle fracture due to hydrogen atoms. The use of UMAT (User Material Subroutine) subroutines and UEL (User Element Subroutine) subroutines to simulate hydrogen-assisted crack propagation behavior (HAC, Hydrogen-assisted cracking) is currently a hot topic in the field of finite element simulation. This paper will summarize the main principles and methods for simulating the hydrogen-assisted crack propagation process using UMAT subroutines and UEL subroutines.

二、模型介绍 II. Model Introduction

UMAT中实现材料的弹性变形过程，其有效应力与二次退化函数有关，详见上一篇《材料脆性断裂有限元模拟的UEL子程序实现方法》：

The elastic deformation process of materials in UMAT is related to the effective stress and the secondary degradation function, see the previous article "UEL Subprogram Implementation Method for Material Brittle Fracture Finite Element Simulation":

$$\hat{\boldsymbol{\sigma}}_0 = \boldsymbol{\sigma} / \left[(1 - \phi)^2 + k \right]$$

材料中的氢扩散满足以下守恒定律: The hydrogen diffusion in materials satisfies the following conservation law:

$$\int_{\Omega} \frac{dC}{dt} dV + \int_{\partial\Omega} \mathbf{J} \cdot \mathbf{n} dV = 0$$

根据高斯散度定理可得上式的强形式: According to Gauss's divergence theorem, the strong form of the above equation can be obtained:

$$\frac{dC}{dt} + \nabla \cdot \mathbf{J} = 0$$

上式对于任意的浓度微分项都满足：The above equation satisfies for any concentration differential term:

$$\int_\Omega \delta C\left(\frac{dC}{dt} + \nabla \cdot \mathbf{J}\right)dV = 0$$

采用散度定理，可得平衡方程的弱形式：By using the divergence theorem, the weak form of the equilibrium equation can be obtained:

$$\int_\Omega \left[\delta C\left(\frac{dC}{dt}\right) - \mathbf{J} \cdot \nabla \delta C\right]dV + \int_{\partial\Omega} \delta C q dS = 0$$

通常认为氢扩散的驱动力来自于氢浓度梯度以及静水应力梯度，因此可表示为：

It is generally believed that the driving force for hydrogen diffusion comes from the hydrogen concentration gradient and the hydrostatic stress gradient, which can be expressed as:

$$\mu = \mu^0 + RT \ln \frac{\theta_L}{1 - \theta_L} - \bar{V}_H \sigma_H$$

其中 μ^0 为参考化学势，R 为气体常数，T 为开氏温度，θ_L 为晶格占有率，$\bar{V}_H$ 为偏摩尔体积，σ_H 为静水应力。氢扩散通量可表示为：

Where μ is the reference chemical potential, R is the gas constant, T is the Kelvin temperature, φ is the lattice occupancy, v is the partial molar volume, and σ is the hydrostatic stress. The hydrogen diffusion flux can be expressed as:

$$\mathbf{J} = -\frac{DC}{RT}\nabla\mu = -D\nabla C + \frac{D}{RT}C\bar{V}_H\nabla\sigma_H$$

将上式代入平衡方程可得：　Substituting the above equation into the equilibrium equation gives:

$$\int_\Omega \left[\delta C\left(\frac{1}{D}\frac{dC}{dt}\right) + \nabla\delta C\nabla C - \nabla\delta C\frac{C\bar{V}_H}{RT}\nabla\sigma_H\right]dV + \frac{1}{D}\int_{\partial\Omega}\delta C q dS = 0$$

令上式为氢扩散过程的不平衡力残差，可离散化为:

Let the above equation be the unbalanced force residual of the hydrogen diffusion process, which can be discretized as:

$$r_i^C = \int_\Omega \left[N_i^T\left(\frac{1}{D}\frac{dC}{dt}\right) + \mathbf{B}_i^T\nabla C - \mathbf{B}_i^T\frac{C\bar{V}_H}{RT}\nabla\sigma_H\right]dV + \frac{1}{D}\int_{\partial\Omega}N_i^T q dS$$

将上式对 C 求导可得切线刚度矩阵为：Taking the derivative of the above equation with respect to yields the tangent stiffness matrix:

$$\mathbf{K}_{ij}^C = \int_\Omega \left[\mathbf{B}_i^T\mathbf{B}_j - \mathbf{B}_i^T\frac{\bar{V}_H}{RT}\nabla\sigma_H N_j\right]dV$$

不平衡力残差第一项可离散为：The first term of the unbalanced force residual can be discretized as:

$$\mathbf{M}_{ij} = \int_\Omega N_i^T\frac{1}{D}N_j dV$$

相场断裂模型采用上一篇《材料脆性断裂有限元模拟的 UEL 子程序实现方法》中所述:

The phase field fracture model adopts the method described in the previous article "UEL Subprogram Implementation Method for Finite Element Simulation of Material Brittle Fracture":

$$r_i^\phi = \int_\Omega \left[-2(1-\phi)N_i H + G_c(\theta_L)\left(\frac{1}{\ell}N_i\phi + \ell\mathbf{B}_i^T\nabla\phi\right)\right]\mathrm{d}V$$

$$\mathbf{K}_{ij}^\phi = \frac{\partial r_i^\phi}{\partial \phi_j} = \int_\Omega \left[\left(2H + \frac{G_c(\theta_L)}{\ell}\right)N_i N_j + G_c(\theta_L)\ell\mathbf{B}_i^T\mathbf{B}_j\right]\mathrm{d}V$$

主要区别在于，临界 Griffith 能量释放率与氢覆盖率相关：

The main difference lies in the fact that the critical Griffith energy release rate is related to the hydrogen coverage:

$$G_c(\theta_L) = G_{c,0}(1 - \chi\theta_L)$$

其中 χ 为材料依赖常数，对于镍可取0.41,氢覆盖率为氢浓度 C 及裂纹表面自由能 $\triangle Q_k$ 相关:

Among them, C is a material-dependent constant, which can be taken as 0.41 for nickel, and the hydrogen coverage is related to the hydrogen concentration and the surface free energy of the crack:

$$\theta_L = \frac{C}{C + \exp\left(\frac{-\Delta Q_k}{RT}\right)}$$

因此可组建线性有限元方程： Therefore, a linear finite element equation can be established:

$$\begin{bmatrix} \mathbf{K}_{ij}^C & 0 \\ 0 & \mathbf{K}_{ij}^\phi \end{bmatrix} \begin{bmatrix} C \\ \phi \end{bmatrix} + \begin{bmatrix} \mathbf{M} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \dot{C} \\ \dot{\phi} \end{bmatrix} = \begin{bmatrix} \mathbf{r}^C \\ \mathbf{r}^\phi \end{bmatrix}$$

采用N-R方法即可求解上式。 The N-R method can be used to solve the above equation.

三、模型交互 Three, Model Interaction

采用三层本构方法，第一层为弹性变形层(UMAT)，第二层为氢扩散层(UEL)，第三层则为相场损伤层(UEL)。在第一层中计算弹性应变能密度及静水应力，通过全局变量传递给第二层；在第二层中计算当前静水应力梯度，进而求解氢浓度分布，通过全局变量传递给第三层；在第三层中计算当前变形条件下的Gc，并使用由全局变量传递的弹性应变能密度，计算当前损伤场的分布；最后，通过全局变量将氢浓度、损伤场传递至UMAT进行可视化。

Adopting a three-layer constitutive method, the first layer is the elastic deformation layer (UMAT), the second layer is the hydrogen diffusion layer (UEL), and the third layer is the phase field damage layer (UEL). In the first layer, the elastic strain energy density and hydrostatic stress are calculated, and then passed to the second layer through global variables; in the second layer, the current hydrostatic stress gradient is calculated, and then the hydrogen concentration distribution is solved, passed to the third layer through global variables; in the third layer, Gc under the current deformation condition is calculated, and the distribution of the current damage field is calculated using the elastic strain energy density passed through global variables; finally, the hydrogen concentration and damage field are passed to UMAT for visualization through global variables.

四、数值模拟 Four, Numerical Simulation

文件输入： File Input:

采用平面应变二次缩减积分单元CPE8R为例，在inp文件中添加如下语句：

Taking the plane strain quadratic reduced integration element CPE8R as an example, add the following statements in the inp file:

-------------------------第二层-------------------------

--------------------------Second Layer--------------------------

*User element, nodes=8, type=U1, properties=1, coordinates=2, variables=4

11

*Element, type=U1, elset=Hydrogen

（单元及其对应节点排序） **(Unit and corresponding node sorting)**

---------------------------第三层---------------------------

---------------------------Third Layer---------------------------

*User element, nodes=8, type=U11, properties=2, coordinates=2, variables=12

4

*Element, type=U11, elset=Phase

（单元及其对应节点排序）　　**(Unit and corresponding node sorting)**

本工作中所需材料参数为：Material parameters required in this work are:

初始 G_c ： 2.7　Initial: 2.7 $MPa \cdot mm$

长度尺度参数 l_c : 0.05　Length scale parameter: 0.05 mm

杨氏模量 E ： 210　Young's modulus: 210 GPa

泊松比 v ： 0.3　Poisson's ratio: 0.3

氢扩散系数 D ： 0.0127　Diffusion coefficient of hydrogen: 0.0127 mm^2/s

偏摩尔体积 $\bar{V}_H$ ： 2000　Partial molar volume: 2000 mm^3/mol

建立了如下的含裂纹几何模型，并设置不同初始氢浓度(0/0.5/0.75/1 $wt.ppm$)：

A crack geometry model as follows has been established, and different initial hydrogen concentrations (0/0.5/0.75/1) have been set:
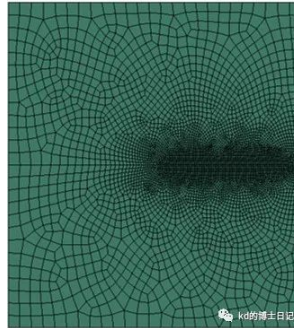

图1 裂纹试样模型及网格分布　Figure 1: Crack specimen model and mesh distribution

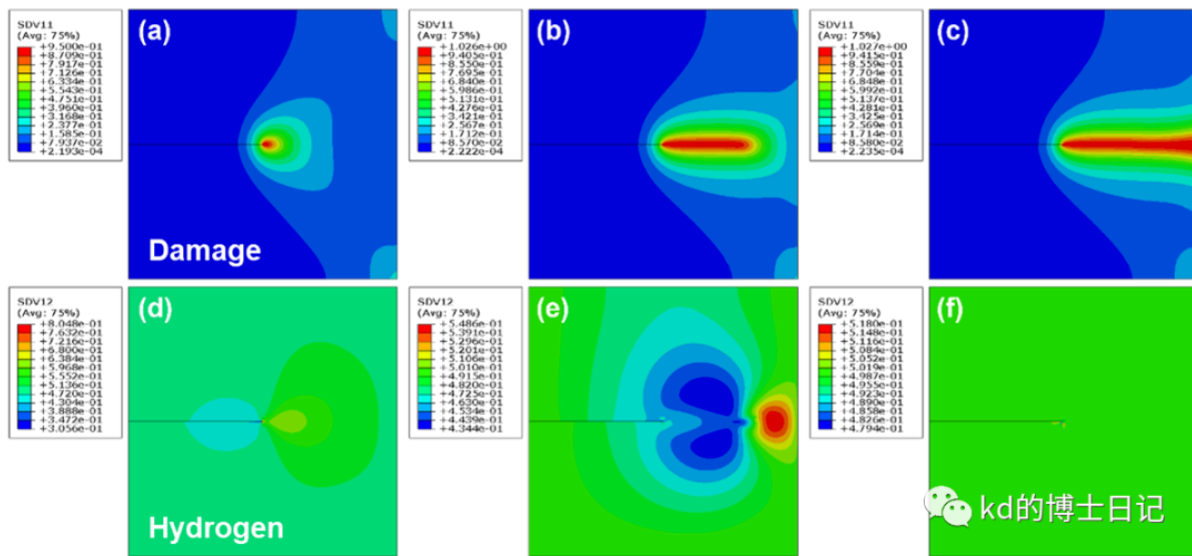计算结果如下： Calculation results are as follows:

图2 模拟结果：(a)(d)-阶段1; (b)(e)-阶段2; (c)(f)-阶段3

Figure 2: Simulation results: (a)(d) - Stage 1; (b)(e) - Stage 2; (c)(f) - Stage 3

如图2所示，随着裂纹的扩展，氢逐渐富集于裂纹尖端部位，进一步弱化尖端部位的 G_c 从而加速裂纹扩展。统计了不同氢浓度条件下CT试样的载荷位移曲线，如图3所示。

As shown in Figure 2, with the propagation of the crack, hydrogen gradually accumulates at the tip of the crack, further weakening the tip and thus accelerating the propagation of the crack. Load-displacement curves of CT specimens under different hydrogen concentration conditions are statistically analyzed as shown in Figure 3.
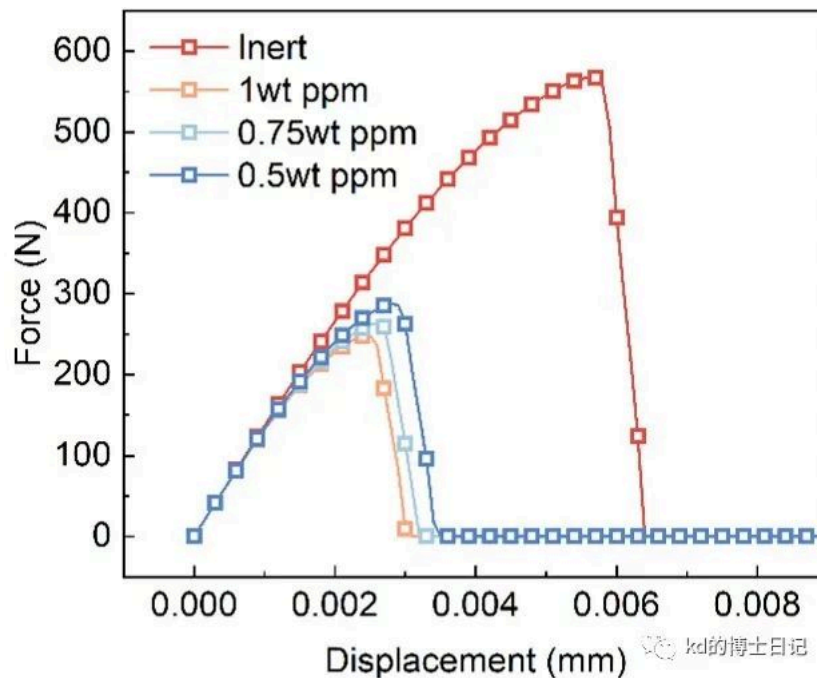

图3 不同边界条件下的载荷位移曲线　Figure 3 Load-displacement curves under different boundary conditions

氢的出现明显降低了样品的承载能力，且该承载能力随着氢浓度的增大而下降。

The presence of hydrogen significantly reduces the load-bearing capacity of the sample, and this capacity decreases with increasing hydrogen concentration.

四、小结 Four, Summary

使用本文所用方法可以预测样品在氢环境下的断裂过程，该方法同样适用于宏观弹塑性模型以及晶体塑性模型。

The method used in this paper can predict the fracture process of the sample in a hydrogen environment, and this method is also applicable to macro-elastic-plastic models and crystal plasticity models.

推荐阅读 Recommended Reading

【专题课程】ANSA HEXABLOCK六面体网格划分专题(完结)…

Wonderful仿真 Wonderful Simulation   ¥399

沉淀原创精品系列全套：XFEM-VCCT-Cohesive-contour等…

沉淀 Precipitation   ¥350 350 RMB

ANSYS必修课_workbench基础操作应用…

大龙猫 🐱 Big Dragon Cat 🐱   ¥188 188 RMB

基于primer和hypermesh的系统分析…

汽车CAE仿真 Automotive CAE sim