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ARTICLE

# Influence of Nickel-Based Alloys' Mechanical Properties on Mechanochemical Effect at Crack Tip in High Temperature Water Environments

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**Abstract:** Mechanochemical effect which is the mechanical and chemical interaction can accelerate the stress corrosion cracking (SCC) in nickel-based alloys used in nuclear power plants. The mechanical property heterogeneity in weld joints will influence the mechanochemical effect indirectly. The influences of yield strength and hardening exponent of nickel-based alloy 600 on the mechanochemical effect of crack tip surface in high temperature water environment were studied by adopting one inch compact tension specimen and finite element method. The influence of elastic and plastic deformation on the mechanochemical effect at crack tip was discussed. The results indicate that the mechanochemical effect is affected by the yield strength. In contrary, the hardening exponent change of alloy 600 has an insignificant influence on mechanochemical effect.

**Key words:** mechanochemical effect; yield strength; hardening exponent; crack tip; finite element

Although important equipments in nuclear power plants, such as reactor pressure vessel, steam generators, and pressurizes, are welded by nickel-based alloys which are heat-resistant and anti-corrosive, the safety of nuclear power is still threatened by stress corrosion cracking (SCC)[1,2]. The quantitative prediction of SCC rate of nickel-based alloys in high temperature water considering the factors affecting SCC has been an important field of safety assessment of nuclear materials. During past 50 years, many SCC mechanisms and prediction models of nickel-based alloys and austenitic stainless steels in high temperature water had been summarized based on a large number of experimental studies[3,4] which provided the guidance for the safety design and operation of nuclear power plants. Although many factors affecting SCC rates have been studied[5,6], it is essential to comprehend the interactions among SCC factors in order to improve the accuracy of SCC model.

As one of the important interactions among SCC factors, the mechanochemical effect which explains the relationship between stress and the electrochemical corrosion environment of SCC, shows that the electrochemical corrosion potential (ECP) of metals will migrate if elastic or plastic deformation occurs[7-9]. It is proved that SCC occurs only in a critical potential range, a tiny disturbance of the potential may change the metal surface status and leads to the variation of corrosion current density and corrosion rates, so the change of stress will accelerate corrosion rates in mechanical and electrochemical aspects simultaneously. The influences of material property differences of nickel-based alloys in heat-affected zone on crack tip stress and strain fields had been studied[10-12], but the indirect influences of material property differences on the mechanochemical effect in SCC process are still unclear. In the present study, the influences of material property differences of nickel based alloy 600 on mechanochemical effect in SCC were discussed by a finite element method (FEM) and sub-model technology.

## 1 Theory Model

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In the system with positive ions and influenced by mechanical and electrical factors simultaneously, the ECP change of metals is different under elastic or plastic deformation. The ECP change of elastic metals is related to the external pressure, and equals to the change of standard electrical potential[7], as shown in the following equation:

$$\Delta\varphi_{\mathrm{E}} = -\frac{\Delta P V_{\mathrm{m}}}{zF} \tag{1}$$

where $\Delta\varphi_{\mathrm{E}}$ is the change of equilibrium electrical potential caused by elastic deformation; $\Delta P$ is external excess pressure experienced by the metal, and it will be denoted by the absolute value of the hydrostatic part of stress tensor, and equals to hydrostatic pressure in Abaqus calculations; $V_{\mathrm{m}}$ is the mole volume of metal; $Z$ is ion valence and $F$ is Faraday's number.

The ECP change in plastic metals is the additional chemical potential of atoms caused by dislocation besides external pressure, and the ECP change caused by dislocation can be calculated by the following equation[7]:

$$\Delta\varphi_{\mathrm{P}} = -\frac{RT}{zF}\ln\frac{\varepsilon}{\varepsilon_0} \tag{2}$$

where $\Delta\varphi_{\mathrm{P}}$ is the change of equilibrium electrical potential caused by plastic deformation; $R$ is gas constant; $T$ is absolute temperature; $\varepsilon$ is the strain of material, and will be instead by equivalent plastic strain in Abaqus calculations; $\varepsilon_0$ corresponds to the onset of strain hardening.

The overall value of mechanochemical effect $\Delta\varphi$ is defined by the standard potential shift which represents a sum of Eq.(1) and Eq.(2):

$$\Delta\varphi = -\frac{1}{zF}\left[RT\ln\frac{\varepsilon}{\varepsilon_0} + \Delta P V_{\mathrm{m}}\right] \tag{3}$$

The Eq.(3) will be used in plastic zone, and in contrary, the Eq.(1) will be used to calculate the ECP change in elastic zone.

## 2 FEM Simulations

### 2.1 Material and specimen model

One inch compact tension specimen (1T-CT) was used in this numerical calculation with the virtual experiment process according to the American Society for Testing and Materials Standard[13]. The geometric shape and the size of 1T-CT specimen are shown in Fig.1. The non linear relationship between stress and strain beyond yield at crack tip of nickel-based alloys is described by Ramberg-Osgood equation in this numerical simulation[14]:

$$\varepsilon = \frac{\sigma}{E} + \alpha\frac{\sigma_0}{E}\left[\frac{\sigma}{\sigma_0}\right]^m \tag{4}$$

where $\varepsilon$ is strain; $\sigma$ is stress; $E$ is Young's modulus of the material; $\sigma_0$ is the yield strength of the material; $\alpha$ is the yield offset and $m$ is the hardening exponent for the plastic deformation.

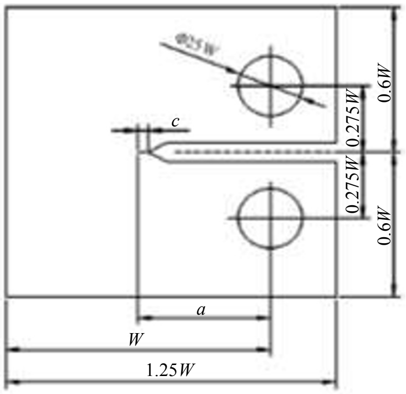

Fig.1 Geometric size of 1T-CT specimen ($W$=50 mm, $a$=0.5$W$, $c$=1.5 mm)

The study was divided into three stages with crack tip stress intensity factor being equal to 7 MPa·m$^{1/2}$ constantly [15]. Firstly, the alloy 600 at 288 °C was used as base metal, the mechanical properties of alloy 600 are given in Table 1 [15]. The yield strength and hardening exponent in Table 1 were regarded as reference value $\sigma_0$ and initial hardening exponent $m_0$, respectively. Secondly, the yield strength of alloy 600 was arbitrarily set to 0.8$\sigma_0$, 0.9$\sigma_0$, 1.1$\sigma_0$, and 1.2$\sigma_0$ with other properties as constant to study the influences of yield strength change on mechanochemical effect. Thirdly, the hardening exponent of alloy 600 was arbitrarily changed to 4.495, 5.495, 7.495 and 8.495 with other properties unchanged to investigate its influence on mechanochemical effect.

The film, which was simplified as $Cr_2O_3$ at alloy 600 surface in PWR (pressurized-water reactor) primary water[16], was assumed dissolving in front of crack and only left on sides of crack. This study focuses on the crack tip without film and the mechanochemical effect only affect the anodic dissolution current[17]. The simulation parameters used in this study are listed in Table 2[15].

**Table 1 Mechanical properties of alloy 600 and passive film in PWR primary water at 288 °C[15]**

| Property | Alloy 600 | Passive film |
|---|---|---|
| Yield strength, $\sigma_0$/MPa | 436 | 810 |
| Young's modulus, $E$/GPa | 189.5 | 140 |
| Yield offset, $\alpha$ | 3.075 | 3.075 |
| Hardening exponent, $m$ | 6.495 | 6.495 |
| Poisson's ratio, $\nu$ | 0.286 | 0.31 |

**Table 2 Parameters used in simulation[15]**

| Parameter | Value |
|---|---|
| Ion valence, $Z$ | 2 |
| Faraday's number, $F$/C·mol$^{-1}$ | 96 485.338 3 |
| Mole volume of alloy 600, $V_{\mathrm{m}}$/cm$^3$·mol$^{-1}$ | 6.749 8 |
| Gas constant, $R$/J·K$^{-1}$·mol$^{-1}$ | 8.314 472 |
| Absolute temperature, $T$/K | 613.15 |